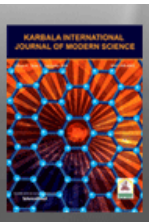


Karbala International Journal of Modern Science

Manuscript 3374

Gas chromatography-Mass Spectrometry (GC-MS), Computational Analysis, and In Vitro Effect of Essential Oils from Two Aromatic Plants, Bubonium graveolens and Launaea arborescens Growing in Southwest Algeria Against Potato Cyst Nematodes

Souad Ziane

Chaouki Selles

Khaldun M. Al Azzam

Bounoua Nadia

Belal O. Al-Najjar

See next page for additional authors

Follow this and additional works at: https://kijoms.uokerbala.edu.iq/home

 Part of the Biology Commons, Chemistry Commons, Computer Sciences Commons, and the Physics Commons

University of Kerbala

Gas chromatography-Mass Spectrometry (GC-MS), Computational Analysis, and In Vitro Effect of Essential Oils from Two Aromatic Plants, Bubonium graveolens and Launaea arborescens Growing in Southwest Algeria Against Potato Cyst Nematodes

Abstract

The study tested the nematicidal effects of essential oils from Bubonium graveolens and Launaea arborescens on the potato cyst nematode Globodera rostochiens. The chemical composition of the essential oils was analyzed using GC-MS. To determine the concentration that killed 50% of the nematode population (LC50), five concentrations of the essential oils were applied to the tested organisms. The effects of essential oils on the hatching of cyst nematode (Globodera rostochiensis sp.) eggs in vitro demonstrated a wide variety of effects ranging from no impact to mild, moderate, and strong effects, which increased dramatically with exposure duration and concentration. All the oils examined were capable of causing Globodera cysts to hatch, although the effects varied depending on the type of oil used, how long it was exposed to, and its concentration. The percentage of nematode mortalities ranged from 7.14 to 78.56% for Bubonium graveolens, 7.14 to 85.71% for Launaea arborescens, and 64.38 to 73.31% for the nematode control. This study investigated the effects of bioactive compounds from Bubonium graveolens and Launaea arborescens plants on the body and the molecular mechanisms underlying cyst nematode egg hatching.

Asteraceae, bionematicide, Bubonium graveolens, Globodera rostochiensis , Launaea arborescens.

Keywords

Asteraceae, bionematicide, Bubonium graveolens, Globodera rostochiensis, Launaea arborescens

Creative Commons License

This work is licensed under a Creative Commons Attribution-Noncommercial-No Derivative Works 4.0 License.

Authors

Souad Ziane, Chaouki Selles, Khaldun M. Al Azzam, Bounoua Nadia, Belal O. Al-Najjar, Ali Al-Samydai, Obada A. Sibai, and El-Sayed Negim

RESEARCH PAPER

Gas Chromatography-mass Spectrometry (GC-MS), Computational Analysis, and *In vitro* Effects of Essential Oils from Two Aromatic Plants, *Bubonium graveolens* and *Launaea arborescens*, Grown in Southwest Algeria Against Potato Cyst Nematodes

Souad Ziane [a,**], Chaouki Selles [a], Khaldun M. Al Azzam [b,*], Bounoua Nadia [c,d], Belal O. Al-Najjar [e,f], Ali Al-Samydai [f], Obada A. Sibai [g], El-Sayed Negim [h,i]

[a] Laboratory of Natural and Bioactive Substances (LASNABIO), Department of Chemistry, Tlemcen, Algeria
[b] Department of Chemistry, Faculty of Science, The University of Jordan, 11942 Amman, Jordan
[c] Normal Higher School of Bechar, Department of Exact Sciences, Laboratory of the Innovation Sponsorship and the Emerging Institution for Graduates of Higher Education of Sustainable Development and Dealing with Emerging Conditions, 8000, Bechar, Algeria
[d] Laboratory of Chemical and Environmental Science (LCSE), 8000, Bechar, Algeria
[e] Department of Pharmaceutical Sciences, Faculty of Pharmacy, Al-Ahliyya Amman University, 19328 Amman, Jordan
[f] Pharmacological and Diagnostic Research Centre, Al-Ahliyya Amman University, 19328 Amman, Jordan
[g] Department of Pharmacy, Faculty of Pharmacy, Al-Zaytoonah University of Jordan, Amman, Jordan
[h] School of Petroleum Engineering, Satbayev University, 22 Satpayev Street, Almaty 050013, Kazakhstan
[i] School of Materials Science and Green Technologies, Kazakh-British Technical University, St. Tole bi, 59, Almaty 050000, Kazakhstan

Abstract

The study tested the nematicidal effects of essential oils from *Bubonium graveolens* and *Launaea arborescens* on the potato cyst nematode *Globodera rostochiens*. The chemical composition of the essential oils was analyzed using GC-MS. To determine the concentration that killed 50% of the nematode population (LC_{50}), five concentrations of the essential oils were applied to the tested organisms. The effects of essential oils on the hatching of cyst nematode (*Globodera rostochiensis* sp.) eggs *in vitro* demonstrated a wide variety of effects ranging from no impact to mild, moderate, and strong effects, which increased dramatically with exposure duration and concentration. All the oils examined were capable of causing *Globodera cysts* to hatch, although the effects varied depending on the type of oil used, how long it was exposed to, and its concentration. The percentage of nematode mortalities ranged from 7.14 to 78.56% for *B. graveolens*, 7.14−85.71% for *L. arborescens*, and 64.38−73.31% for the nematode control. This study investigated the effects of bioactive compounds from *B. graveolens* and *L. arborescens* plants on the body and the molecular mechanisms underlying cyst nematode egg hatching.

Keywords: *Asteraceae*, Bionematicide, *Bubonium graveolens*, *Globodera rostochiensis*, *Launaea arborescens*

1. Introduction

Bubonium graveolens (Forsk), a member of the Asteraceae family, is a significant Saharan medicinal plant known for its fragrance and medicinal properties. It is commonly found in dry and semiarid regions. It is used to treat the gastrointestinal tracts, treating fever, cephalic pains, bronchitis, and anti-inflammatory medications. Recently, it has been used as a botanical fungicide with antibacterial and hypoglycemic properties [1]. Asteraceae is a broad family that includes 54 Launaea species, 12 of

Received 30 April 2024; revised 25 September 2024; accepted 28 September 2024.
Available online 23 October 2024

* Corresponding author.
** Corresponding author.
E-mail addresses: souadziane09@gmail.com (S. Ziane), azzamkha@yahoo.com (K.M. Al Azzam).

https://doi.org/10.33640/2405-609X.3374
2405-609X/© 2024 University of Kerbala. This is an open access article under the CC-BY-NC-ND license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

which are in Algeria. *Launaea arborescens* (Batt) Murb is endemic and widespread in southwestern Algeria, with multiple geometric branches, leaves reduced to alternate spines, and a yellow bloom. It can thrive in saline soil and withstand high temperatures in desert areas [2]. Potato root nematodes (*Globodera rostochiensis* (Wollenweber) and Behrens) and *Globodera pallida* (Stone) Behrensare are one mm long roundworms belonging to the genus Globodera and include approximately twelve species [3]. Moreover, potato cyst nematodes induce plant growth retardation, root harm, and early senescence at high population densities [4]. The cyst nematodes (CNs) of the genus Globodera (GLO) are the world's second most commercially and scientifically significant plant-parasitic nematode (PPN) group [5]. Essential oils (EOs), also known as aromatic oils found in plants and consisting of terpenoids, aromatic phenols, oxides, ethers, alcohols, esters, aldehydes, and ketones, have been utilized for domestic and pharmaceutical purposes for centuries. Recently, there's been a growing interest in using them as natural insecticides to control various plant nematodes and animal parasites [6,7]. Numerous studies have shown the effectiveness of EOs from various plant species, focusing mostly on Meloidogyne species and potato cyst nematodes [8]. In addition, how essential oils and plant extracts affect the migration, mortality, and hatching of Meloidogyne incognita plants has been investigated [9]. To determine which species and fragrant plants in the Asteraceae family have the best nematicidal properties, researchers have tested the nematicidal effects of EOs from 27 different species and chemotypes on the root-knot nematode *Meloidogyne javanica* [10]. EOs have also been shown to have nematocidal effects on Meloidogyne incognita on tomato plants and on the psychrophilic Panagrolaimus sp. (Nematoda: Panagrolaimidae) [6,11]. The constituents of EOs can act directly, inhibiting nematode hatching and increasing the mortality of nematodes in the soil, or if they are absorbed by plants, they may alter the composition of the root exudates, inhibiting the nematodes' ability to locate the roots and inhibiting the attraction of the pathogen [12]. Plant EOs have gained popularity as effective pesticidal compounds due to their ecofriendly, biodegradable nature and minimal impact on plants and human health. EOs play crucial roles in pollination, symbiotic relationships, and cell wall structure. Steam distillation is the most common method because of its simplicity and cost-effectiveness [13–15]. EOs have nematicidal activity due to their terpenes, which contain oxygen and disrupt plasma membrane permeability. These terpenes can cause cytotoxic activity, leading to cell death in organisms such as plant parasitic nematodes. Their chemical structure can induce mitochondrial membrane depolarization, apoptosis, DNA damage, and cell death, highlighting the importance of considering factors such as plant phenological age, harvested material humidity, and extraction methods [16]. Furthermore, EOs contain organosulfur compounds, phenols, and aldehydes that have nematicidal effects on nematodes, influencing their neurotransmission and chemosensing functions [17,18]. Phenylpropanoids in plant EOs show promising results against nematodes by impeding the V-ATPase enzyme, which is crucial for nematode nutrition, osmoregulation, and reproduction. Catani et al. (2024) [19] summarized nematode targets, botanical species of essential oil, the effect on nematodes, and the duration of exposure.

The medicinal plant *L. arborescens* has the capacity for important propagation. *L. arborescens* is commonly found in association with various other species throughout the southwestern region of Algeria, extending from Wadi Namous to the Karzaz area [20]. It spans from northern Africa to the Central Asian desert, although it is particularly prevalent in southwest Algeria and southeast Morocco (where it is known as Tafss). In traditional Saharan medicine, the entire plant—including blooms and leaves—is used to treat a variety of illnesses, including bronchitis, digestive system problems, fever, and cephalic aches. According to Said et al., 2016 [21], *B. graveolens* also has antibacterial, antioxidant, and antifungal properties. These plants may be grown in many different ways to guard crops that are susceptible to parasitic worms. However, the majority of related studies in this field originate from the planet's tropics [22]. For crop protection and higher yields, pesticide usage in agriculture is essential. However, pesticides might also negatively affect human health [22]. Natural bioactive substances are advantageous for the environment and consumer health in this situation, and they serve as fresh targets for the development of innovative techniques to manage plant-parasitic nematodes [23]. The goal of the present study was to investigate and analyze the chemical composition of the EOs of the aromatic herbs *B. graveolens* and *L. arborescens* using gas chromatography-mass spectrometry (GC-MS) and to assess the nematostatic effectiveness of the extracts for hatching egg masses of the cyst nematode (*G. rostochiensis*). The developed GC-MS methods include microwave-assisted extraction, hydrodistillation, and direct headspace analysis in two different stationary phases columns. In total, 110 volatile compounds were identified, 90

of which were identified via Rxi-5MS and 78 of which were identified via HP-INNOWAX. Furthermore, the molecular mechanisms that support the hatching of cyst nematode (*G. rostochiensis* sp.) eggs from the fragrant herbs *B. graveolens* and *L. arborescens* have been studied.

2. Materials and methods

2.1. Materials

2.1.1. Plant materials

The aerial parts (leaves and stems) of *B. graveolens* and *L. arborescens* were collected in April 2020 from two cities in southwestern Algeria (Lahmer and Boukais). The samples were harvested after the flowering period. EOs were extracted using the hydro-distillation method using Clevenger equipment. For 3 h, 100 g of fresh aerial parts were extracted with distilled water, until the entire sample was immersed in a glass flask connected to Clevenger-type equipment [24].

2.1.2. Potato cyst nematodes G. rostochiensis

Nematodes were extracted at the National Institute of Plant Protection (INPV), El Harrach, Algiers, Algeria. All the soil samples used in this study consisted of different subsamples collected from different infested areas in *Chlef*, Algeria.

2.1.2.1. Soil preparation. The sample taken for analysis was preceded by the removal of large stones and plant debris, reduction of clods, and homogenization of the product. A mesh screen of 4 or 5 mm was used to complete the preparation [25].

2.1.2.2. Extraction of masses from eggs. Fenwick (Fig. 1) was used to extract the samples. The apparatus consisted of a container with a tapered top and a collar with a sloped outer edge that collected spillage and sent it away from an exit. The can has a bottom drain plug and an internal base that slopes. After being passed through a 1-mm sieve, the soil sample was placed in the can that was held above the container by a long-stemmed funnel. The can is then first filled with water. The organic material will immediately rise to the surface and spill over onto the collar before being collected on two sieves with 840 μm and 250 μm holes. This stage will include gathering the bulk of the cysts present in the soil sample. Water is immediately pumped through a lengthy glass or metal tube once the funnel over the can is removed to dissolve the dirt at the bottom of the can. To mix the sediment and free any trapped

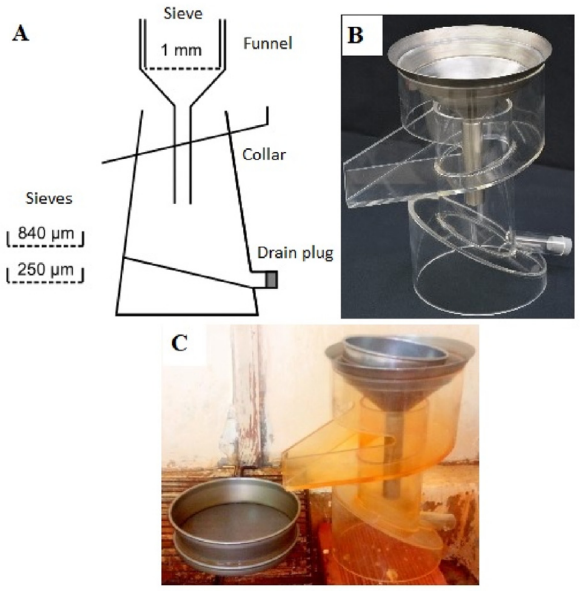


Fig. 1. Extraction method. A: Vertical-section diagram of the Fenwick can. B: Real Fenwick (new one). C: Fenwick with sieves after usage in our lab.

cysts, the tube was inserted deep into the container and left there for approximately 1 min. For further processing, the cysts were collected on a sieve with a 250 μm aperture [26].

2.1.2.3. Isolation of cysts. Cyst isolation can be accomplished in two ways. First, based on the idea that dried cysts float, several methods are used. An empty beaker, flask, or white dish was used to hold the dried soil sample. The solution was stirred. Depending on the type of soil, the water will clear within 30 s to a few minutes, exposing only the cysts and floating organic detritus. Cysts can be manually removed with a brush after the addition of a drop of detergent, which causes the cysts to travel to the edge [27]. The second technique, referred to as the "Manual Method," involves performing isolation using a brush and syringe while utilizing a binocular microscope [28].

2.2. In vitro *bioassay*

The effectiveness of bioactive compounds extracted from the two plants on cyst nematodes (*G. rostochiensis*) was tested *in vitro*. The dishes were 5 cm in diameter and contained 5 mL of biological solution and distilled water.

To obtain the recommended concentrations (biological solution) and nematicide (10% VETACUR) for the control, essential oil solutions (10% ethanol,

v/v) were diluted with water containing 0.3% (Tween 20, v/v%). Ten cyst nematode egg masses in 10 μL of water were subjected to essential oil solutions of 50, 100, 200, 400, and 800 μL mL^{-1} and incubated at 25 °C for three days before hatching. The mortality of juveniles and eggs was monitored every day for three days [29]. When mechanically prodded and observed under a binocular microscope, the nematodes were deemed dead if their bodies stayed straight or did not move [30]. Mortality percentages were determined from three repetitions. The results are expressed as the percent mortality and were recorded after 24, 48, and 72 h. After the egg masses were treated with bioactive compounds, the mortality rate of these cysts was observed using a stereomicroscope.

2.3. Gas chromatography-mass spectrometry (GC-MS)

The oil was analyzed using GC-MS. Hewlett-Packard Agilent gas chromatography (model 6890) plus 2 split/splitless injectors coupled with a single quadrupole mass spectrometer (Hewlett-Packard Agilent model 5973) was used throughout the analysis. A fused silica capillary HP-5ms GC column was used with the following dimensions: 30 m × 0.25 mm × 0.25 μm (stationary phase: 5% phenyl-methyl-polysiloxane). Helium as a carrier gas was used at a constant flow rate of 0.6 mL/min. The injector, GC-MS interface, and ion source temperatures were 250 °C, 270 °C, and 230 °C, respectively. Essential oil samples (0.2 μL) were injected neatly at a split ratio of 1:80. The column temperature was held at 45 °C for 8 min and then raised to 250 °C at 2 °C/min, and finally isothermal mode for 10 min operating in electron impact mode at 70 eV was used. The identity of the chemical components was determined by comparison of their mass spectral profiles with those stored in the MS library (NIST and Wiley 7N library) and the literature. Without using any correction factors, the percentage of composition of the detected compounds was determined from the GC peak area. The essential oil analysis is the mean value of three replications.

2.4. Molecular docking

In this study, we sought to gain deeper insights into the molecular mechanisms underlying the hatching of eggs of the cyst nematode (*G. rostochiensis* sp.) from the aromatic herbs *B. graveolens* and *L. arborescens*. To elucidate the underlying mechanism, molecular docking simulation screening was conducted with AutoDock Vina 1.1.2 with tacrine(8)-4-aminoquinoline serving as a control for comparative analysis [31,32]. To facilitate these simulations, we utilized the crystal structure of the *Tetronarce californica* acetylcholinesterase enzyme (PDB ID: 1ODC) [33].

The preparation of both proteins and ligands for the docking simulations was carried out using AutoDockTools 1.5.7. Initially, the enzyme crystal structure was loaded into AutoDockTools 1.5.7, polar hydrogens were added, and Kollman charges were assigned further increasing the accuracy of the protein representation. Each ligand molecule was subsequently loaded separately, and Gasteiger charges were assigned, considering the specific chemical properties of each ligand. Furthermore, a grid box with a default grid spacing of 0.375 Å was established. The center of this grid box was defined at coordinates 1.670265 (x), 64.936618 (y), and 68.216176 (z), ensuring an appropriate spatial context for the docking calculations.

Finally, the actual docking simulations were executed using default parameters, and a Lamarckian genetic algorithm was employed across 100 num modes. The results were subsequently analyzed by examining the AutoDock Vina log files. Of particular interest were the lowest energy of binding (LEB) values for each ligand, with a focus on identifying the conformer displaying the most favorable binding energy. To further refine our selection, we considered the conformer with the highest number of clusters, thus ensuring the robustness of our choice of ligand conformations. These selected conformers were then exported and visualized using BIOVIA Discovery Studio Visualizer 16.1, providing insights into the binding interactions of the identified compounds, and the reference compound tacrine(8)-4-aminoquinoline, with the acetylcholinesterase enzyme.

2.5. Data analysis

The corrected mortality rates of *B. graveolens* and *L. arborescens* were determined via probit analyses. All the assays were performed three times. Three replicates of each treatment were used in the tests, which were conducted in a completely random experimental setup with one glass Petri dish filled with potato roots in each experimental unit.

2.6. Statistical analysis

The mortality percentages of nematodes (hatching of eggs) were corrected by removing the natural death in the control [34] and calculated according to Schneider-Orelli's formula [35].

$$\text{Corrected mortality } \% = \frac{\text{Mortality } \% \text{ in treatment} - \text{Mortality } \% \text{ in control}}{100 - \text{Mortality } \% \text{ in control}} \times 100$$

The resulting mortality data were translated into percentages and subjected to regression analysis with XLSTAT®.

3. Results and discussion

The results showed that nematicidal activity varied among exposure times and concentrations, where the concentrations and exposure times of the oil extracts of both plants tested increased. The inhibition of egg hatching by *B. graveolens* extracts strongly inhibited egg hatching in *G. rostochiensis* eggs after 72 h. The best nematicidal activity (85.71%) was observed for the oil extract of *L. arborescens* at a concentration of 800 μL mL^{-1} after 72 h (Table 1), and at the same concentration, 78.56% was obtained for *B. graveolens.*

The nematicidal activity of the EOs from *B. graveolens* was greater than that of the EOs from *L. arborescens* at all concentrations. Chemical treatment caused 73.71% mortality of egg masses after 72 h (Table 1).

At a dose of 400 μL mL^{-1} after 48 h, the percentage of corrected mortality was 64.28% for the essential oil of *B. graveolens* and 42.85% for that of *L. arborescens*. After 72 h, the mortality rate of arborescents caused by *G. rostochiensis* increased to 57.14% (Table 1). For low doses of 100 μL mL^{-1} and 200 μL mL^{-1}, after 72 h of exposure, the mortality rates exceeded 35% for both plants at a dose of 200 μL mL^{-1}, and the mortality rate of *B. graveolens* exceeded 50% after 72 h of exposure. At low doses (50 μL mL^{-1}), the mortality after 72 h of exposure was less than 10%, regardless of the oil tested (Table 1).

The present study is one of the first biological prospective studies on the use of EOs from the saharien medicinal plant EOs against the cyst nematode *G. rostochiensis*.

Furthermore, this study improves the understanding of several plant species that are naturally nematicidal. The significant increases in both concentration of EOs and time with increasing mortality are shown in Figs. 2 and 3 for both *B. graveolens* and *L. arborescens*, respectively. The results shown in Fig. 3 are supported by the study of Khan et al., 2019, who demonstrated that the death of juveniles was closely related to the concentration and duration of exposure [36]. These results were also confirmed by

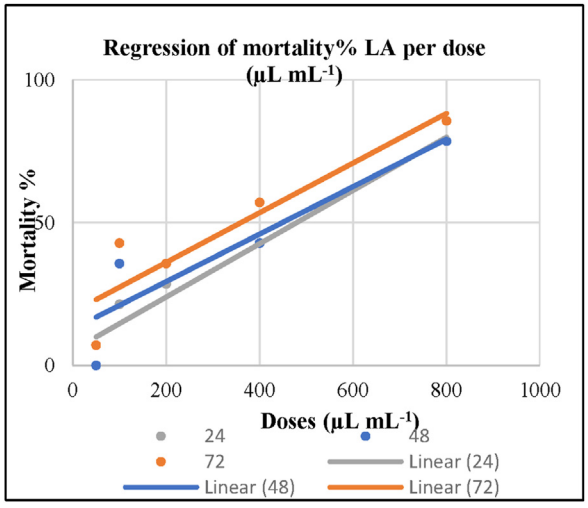
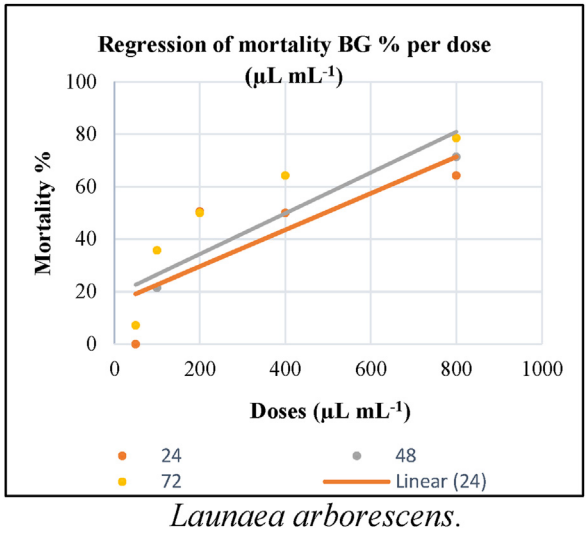


Fig. 2. Mortality regression of the essential oils of Bubonium graveolens.

Table 1. In vitro *bioassay of essential oils of* Bubonium graveolens *and* Launaea arborescens *at different doses.*

Tested Plants	Exposure Time (hours)	Corrected Mortality* Percentage (%)				
		Dose 50 (μL mL^{-1}) ± SD	Dose 100 (μL mL^{-1}) ± SD	Dose 200 (μL mL^{-1}) ± SD	Dose 400 (μL mL^{-1}) ± SD	Dose 800 (μL mL^{-1}) ± SD
Bubonium graveolens	24	0 ± 1.5	21.42 ± 0.642	50.56 ± 3.556	49.99 ± 3.499	64.28 ± 4.928
	48	7.14 ± 0.786	21.42 ± 0.642	49.98 ± 3.498	64.28 ± 4.928	71.42 ± 5.642
	72	7.14 ± 0.786	35.72 ± 2.072	49.98 ± 3.498	64.28 ± 4.928	78.56 ± 6.356
Launaea arborescens	24	0 ± 1.5	21.42 ± 0.642	28.56 ± 1.356	42.85 ± 2.785	78.56 ± 6.356
	48	0 ± 1.5	35.72 ± 2.072	35.71 ± 2.071	42.85 ± 2.785	78.56 ± 6.356
	72	7.14 ± 0.786	42.86 ± 2.786	35.71 ± 2.071	57.14 ± 4.214	85.71 ± 7.071
Control (Tween + Ethanol)	24	30 ± 2.7	–	–	–	–
	48	30 ± 2.7	–	–	–	–
	72	30 ± 2.7	–	–	–	–
Nematicide (control)	24	64.38 ± 6.138	–	–	–	–
	48	69.26 ± 6.626	–	–	–	–
	72	73.31 ± 7.031	–	–	–	–



Launaea arborescens.

Fig. 3. Mortality regression of essential oils of Launaea arborescens.

Sellami et al. (2010), using EOs from plants of the Asteraceae family [29].

For each oil tested, the mortality at low doses (50 mL mL^{-1}) was less than 10% after 72 h (Table 1); this result was illustrated by Sasanelli et al., 2020, who demonstrated that the hatching percentages were much lower at two concentrations (18 and 36 g/mL) (10.0% and 6.4%, respectively) [37]. On the other hand, the essential oil of *L. arborescens* did not induce resistance to *G. rostochiensis* at a concentration of 50 µL/mL (Table 1), and this result was confirmed by Amora et al. (2017), using the EOs of *Artemisia absinthium* on *M. javanica* [38].

By hatching egg masses, EOs from two plant species have been demonstrated to have the same nematocidal impact on cyst nematodes, as was also observed in the research of Barbosa et al. (2010), who reported the hatching of eggs (root-knot nematodes) using essential oils from Asteraceae plants [39].

For the controls, the majority of the hatched eggs were from biological solutions (tween and ethanol), and for the treatment control, a concentration of 50 µg mL^{-1} of VETACUR was used. The percentage of mortality was greater than 60% and exceeded 72% after 24 and 72 h, respectively.

EOs tested in this study have different modes of action on the hatching of eggs because the results reveal different nematicidal activities, such as larvicidal, ovicidal, and nematicidal activities. Larvicidal activity was found only in the *B. graveolens* samples (Fig. 4).

3.1. Calculation of the lethal concentration (LC_{50})

The values of the LC_{50} calculations revealed that these values decreased with increasing exposure

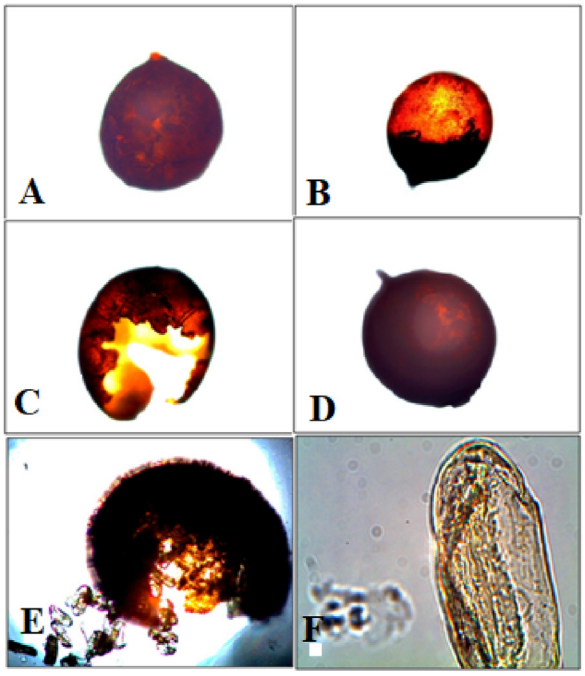


Fig. 4. Different aspects of cysts observed under a stereoscopic microscope: A: egg mass during hatching; B: accumulation inside egg mass; C: total hatching of egg mass in the absence of egg and L2 (larval stage); D: no hatching of egg mass (nematode-static activity); E: the hatching of egg mass with the appearance of egg and the absence of L2 (larval stage); (ovicidal activity). F: juvenile inside the egg. Magnification 40×; F 60×.

period. For example, for *Bubonium gravelens*, the LC_{50} values obtained after 24, 48, and 72 h were 97.85, 97.90, and 89.70 µL mL^{-1}, respectively. However, the correlation coefficient was significant because the R^2 was greater than 0.795 (Table 2).

3.2. Gas chromatography-mass spectrometry (GC-MS)

EOs are complex substances that must be identified using various methods to ensure customer safety, quality, and fair trade. Thus, many instrumental approaches, including organoleptic, physical, chemical chromatographic, and spectroscopic methods, are available. Furthermore, methods such as differential scanning calorimetry (DSC), thermogravimetric analysis (TGA), Fourier transform near-infrared (FTNIR) spectroscopy, and Fourier transform infrared (FTIR) spectroscopy have been investigated for the extraction of chemical components from EOs. According to the literature, GC-MS is commonly used to characterize EOs. This method allows the extraction of tiny essential oil constituents (volatile compounds) based on their boiling points [40].

GC-MS analysis revealed that the EOs of *B. graveolens* contained interesting bioactive

Table 2. At the lethal concentration (µL/mL), 50% of the mortalities were caused by the essential oils of Bubonium graveolens *and* Launaea arborescens.

Exposition Time (Hours)	Plants	Equation	[a]R^2	[b]LC_{50} (µL/mL)
24	*Bubonium graveolens*	Y = 0.0933x + 5.3521	0.9505	97.85
	Launaea arborescens	Y = 1.7143x + 0.615	0.9475	354.81
48	*Bubonium graveolens*	Y = 0.0831x + 12.8	0.8234	97.90
	Launaea arborescens	Y = 1.5707x + 0.0717	0.8573	316.22
72	*Bubonium graveolens*	Y = 0.087x + 18.749	0.8460	89.70
	Launaea arborescens	Y = 1.8213x + 0.6965	0.8853	199.52

Keynotes to abbreviations:
[a] R^2: Regression coefficient.
[b] LC_{50}: Lethal concentration.

compounds. Table 3 shows a summary of the names of the compounds (63 compounds), molecular weights, retention times, and area percentages corresponding to the probabilities related to the NIST library. Table 4 shows the results of the GC-MS analysis of the EOs of *L. arborescens*, which contained 66 compounds. The natural product is extracted from plants, and the method of extraction is important with sophisticated apparatuses such as gas chromatography coupled with mass spectrometry. Typical chromatograms of the EOs obtained for both *B. graveolens* and *L. arborescens* (chromatograms are not shown and will be provided upon request).

This analysis is useful for understanding the efficiency of the *in vitro* effects of EOs from two aromatic plants, *B. graveolens* and *L. arborescens,* on potato cyst nematodes induced by different chemicals.

Tables 3 and 4 show the list of compounds whose GC-MS concentration was not less than 0.1% of the total peak concentration. According to Table 3, fifty-one (not less than 0.1%) components were identified in the essential oil, which represented approximately 99.03% of the total composition of *B. graveolens*. According to Table 4, fifty-nine (not less than 0.1%) components were identified in the essential oil, accounting for approximately 99.52% of the total composition of *L. arborescens*. The major constituents of *B. graveolens* and *L. arborescens* oil were characterized as 1-undecene (37.18%) and 2-[(2*R*,4*aR*,8*aS*)-4*a*-methyl-8-methylidene 1,2,3,4,5,6,7, 8*a*-octahydronaphthalen-2-yl]propan-2-ol (22.40%), respectively.

3.3. Molecular docking

Molecular docking screens were conducted to elucidate the molecular mechanisms underlying the hatching of cyst nematode (*G. rostochiensis* sp.) eggs from the analyzed compounds from the aromatic herbs *B. graveolens* and *L. arborescens on* the acetylcholinesterase enzyme. To validate the docking procedure, the cocrystal structure of tacrine(8)-4-aminoquinoline was redocked, yielding a similar docking pose, as depicted in Fig. 5. As presented in Table 5, the ligand binding energies (LBEs) of the analyzed compounds from the aromatic herb *B. graveolens* showed close binding affinities toward enzymes ranging from −9.3 to −9.6 kcal/mol, whereas the reference compound tacrine(8)-4-aminoquinoline had a binding affinity of −11.0 kcal/mol. LBEs and binding interactions of the top-ranked *B. graveolens* compounds identified. For comparative purposes, tacrine(8)-4-aminoquinoline, a known control molecule, was also included in the analysis. Notably, the top-ranked *B. graveolens* compounds (N-benzyl-N-ethyl-p-isopropylbenzamide, bicyclo [4.4.0]dec-1-ene, 2-isopropyl-5-methyl-9-methylene, and naphthalene,1,2,3,4,4a,7-hexahydro-1,6-dimethyl-4-(1-methylethyl)) exhibited significantly lower binding energies (−9.3 to −9.6 kcal/mol) than did tacrine(8)-4-aminoquinoline (−11.0 kcal/mol). This finding suggested potentially closer binding affinities and potential effects on biological activity.

For the compounds analyzed from the aromatic herb *L. arborescens,* as presented in Table 6, the LBEs for the analyzed compounds from the aromatic herb *L. arborescens* showed similar binding affinities toward the enzyme, ranging from −9.0 to −9.6 kcal/mol, compared with the reference compound tacrine(8)-4-aminoquinoline, which had a binding affinity of −11.0 kcal/mol. The LBEs and binding interactions of the top-ranked *L. arborescens* compounds were identified. For comparative purposes, tacrine-(8)-4-aminoquinoline, a known control molecule, was also included in the analysis. Notably, the top-ranked *L. arborescens* compounds (NDelta-cadinene, alpha-cubebene, and alpha amorphene) exhibited significantly lower binding energies (−9.0 to −9.6 kcal/mol) than did tacrine(8)-4-aminoquinoline (−11.0 kcal/mol). This finding suggested potentially closer binding affinities and potential effects on biological activity.

Table 3. GC-MS analysis of Bubonium graveolens *essential oil.*

No.	CAS	Name of compound	Molecular weight (g/mol)	RT (min)	Kovats index	Area %
1	6728-26-3	*trans*-2-hexenal	98.14	3.3885	943	0.1054
2	2177-78-8	Methyl 3-methylpentanoate	130.19	4.1831	977	0.0744
3	2412-80-8	4-methyl-pentanoic acid methyl ester	130.18	4.4303	987	0.0975
4	2867-05-2	4-methyl-1-propan-2-ylbicyclo[3.1.0]hex-2-ene	150.22	5.5722	1031	0.0268
5	7785-26-4	(1R,5R)-4,7,7-trimethylbicyclo[3.1.1]hept-3-ene	152.24	5.843	1041	2.1002
6	79-92-5	2,2-dimethyl-3-methylidenebicyclo[2.2.1]heptane	136.23	6.4081	1062	0.1559
7	127-91-3	β-pinene	136.24	7.9914	1220	0.9042
8	21195-59-5	1,5,8-p-mentatriene	134.22	9.0627	1258	0.0387
9	14947-20-7	Octa-2,4,6-triene	108.18	9.4218	1271	0.7219
10	99-83-2	2-methyl-5-propan-2-ylcyclohexa-1,3-diene	136.24	9.928	1289	0.1035
11	25155-15-1	Cymene	134.21	11.4348	1208	0.1989
12	5989-54-8	(S)-(−)-limonene	136.23	11.5996	1210	0.2439
13	78-70-6	Linalool	154.25	17.8507	1253	0.3192
14	4501-58-0	2-[(1R)-2,2,3-trimethylcyclopent-3-en-1-yl]acetaldehyde	152.24	18.6924	1259	0.1587
15	55887-81-5	1,3-dichlorocycloheptane	167.01	19.9109	1267	0.3384
16	1462-03-9	1-methylcyclopentan-1-ol	100.16	20.6819	1273	0.2643
17	108-47-4	2,4-dimethylpyridine	107.15	22.8539	1288	0.9532
18	40087-62-5	1,3-cis,5-cis-octatriene	108.18	24.7964	1303	0.1541
19	507-70-0	1,7,7-trimethylbicyclo[2.2.1]heptan-2-ol	154.25	25.6616	1315	0.2323
20	99-48-9	2-methyl-5-(1-methylethenyl)-2-cyclohexen-1-ol	152.23	26.8506	1333	0.1067
21	33522-69-9	2,6,6-trimethyl-bicyclo[3.1.1]hept-2-en-4-ol acetate	194.27	28.8401	1362	12.1199
22	5655-61-8	L-bornyl acetate	196.29	29.8172	1376	0.3125
23	103-90-2	4-acetamidophenol	151.16	31.4359	1400	0.0628
[c]24	696-18-4	1-phenylaziridine	119.16	32.5660	1418	0.9109
25	108287-14-5	1-formyl-2,2,6-trimethyl-3-cis-(3-methylbut-2-enyl)-5-cyclohexene	220.35	33.2017	1428	0.0657
26	103619-06-3	(Z)-8-hydroxylinalool	170.25	37.0689	1488	0.2084
27	3217-94-5	Cyclopentane carboxamide	113.16	37.6517	1497	0.1197
28	6753-98-6	(1*E*,4*E*,8*E*)-2,6,6,9-tetramethylcycloundeca-1,4,8-triene	204.35	39.7648	1532	0.2544
[a]29	107-50-6	Tetradecamethylcycloheptasiloxane	519.08	41.2069	1555	0.0582
[d]30	5144-20-7	3-methoxy-6-azaestra-1,3,5(10),6,8-penten-17-one	281.35	41.7661	1565	0.2701
31	14901-07-6	β-ionone,4-(2,6,6-trimethyl-1-cyclohexenyl)-3-buten-2-one	192.29	42.4489	1576	0.1016
32	489-40-7	(+)-p-gurjunene	204.35	43.6437	1596	0.0893
33	5437-98-9	p-acetoacetanisidide	204.35	44.1853	1605	0.924
34	110528-54-6	Methyl 2-oxo-1-propylcyclopentane-1-carboxylate	184.23	44.8092	1616	0.594
35	128850-52-2	5-amino-4-carbamoyl-3(1H,2H)-pyrazolone	142.00	45.9864	1636	0.9288
36	821-95-4	1-undecene	154.29	48.6705	1683	37.1823
37	70187-91-6	2,6-dimethyl-1,6-heptadien-4-ol acetate	182.26	49.9301	1706	16.9143
38	502-61-4	α-farnesene	204.36	50.3068	1712	0.405
39	5417-74-3	3-methyl-5-(2,6,6-trimethyl-cyclohex-1-enyl)- pent-1-yn-3-ol	222.37	50.4658	1715	0.3514
40	16728-99-7	Naphthlene,1,2,3,4,4a,7-hexahydro-1,6-dimethyl-4-(1-methylethyl)	204.35	50.7542	1721	0.3771
41	1000132-13-0	α-methyl-α-[4-methyl-3-pentenyl]oxiranemethanol	170.25	51.1780	1728	0.8185
42	150320-52-8	Bicyclo[4.4.0]dec-1-ene, 2-isopropyl-5-methyl-9-methylene	204.35	51.6253	1737	1.4473
43	6975-94-6	3,5-dimethylcyclohex-1-ene-4-carboxaldehyde	138.21	52.4141	1751	9.6315
[a]44	541-02-6	Decamethylcyclopentasiloxane	370.77	53.0557	1763	1.0543
[e]45	10586-16-0	2,4-bis[(trimethylsilyl)oxy]benzoic acid trimethylsilyl ester	370.66	53.5207	1772	0.707
46	3242-08-8	(1S,2S)-1-ethenyl-1-methyl-4-propan-2-ylidene-2-prop-1-en-2-ylcyclohexane	204.36	54.1328	1783	0.2479
47	470-82-6	1,3,3-trimethyl-2-oxabicyclo[2.2.2]octane	170.25	54.4625	1789	0.5894
48	18631-68-0	3-methyl-3a,4,5,6,7,7a-hexahydro-1H-inden-1-one	166.22	54.8156	1795	0.297
49	5989-27-5	R(+)-limonene	136.23	55.8457	1815	0.3821
[b]50	13278-00-7	1-deuterioformyl-2-methoxybenzene	137.16	57.2113	1841	3.1694
51	17225-41-1	Methyl-3-benzoxy-12-ketocholanate	124.00	58.0589	1858	0.0997
52	932-66-1	1-(cyclohexen-1-yl)ethanone	124.18	60.6370	1908	0.2437
[a]53	556-71-8	Octadeamethyl-cyclononasiloxane	667.39	61.4434	1925	0.3438
54	1450-72-2	1-(2-hydroxy-5-methylphenyl)ethanone	150.17	62.6206	1948	0.2044
55	80-57-9	4,6,6-trimethylbicyclo[3.1.1]hept-3-en-2-one	150.22	63.0915	1958	0.2407
56	313956-40-0	1-(6,6-dimethylbicyclo[3.1.0]hex-2-en-2-yl)ethanone	150.22	66.582	1998	0.1214
[a]57	18772-36-6	Eicosamethyl-cyclodecasiloxane	741.54	68.9129	1994	0.1258
[a]58	556-71-8	Octadeamethyl-cyclononasiloxane	667.39	81.9625	1974	0.085

(*continued on next page*)

Table 3. (continued)

No.	CAS	Name of compound	Molecular weight (g/mol)	RT (min)	Kovats index	Area %
59	17367-38-3	1,1'-[1,3-propanediylbis(oxy)]bisoctadecane	581.05	90.4797	1961	0.1665
[a]60	556-71-8	Octadeamethyl-cyclononasiloxane	667.39	98.3554	1949	0.1046
61	15089-22-2	N-benzyl-N-ethyl-p-isopropylbenzamide	281.39	103.1702	1942	0.0973
[f]62	1000162-19-6	Chromium, tricarbonyl-.eta.-6-(12-methyl-2-(trimethylsilyloxy)-tricyclo[8.3.0.0(3,8)]trideca-3,5,7-triene-11,13-dione)	439.46	107.6967	1935	0.1011
[a]63	018772-36-6	Eicosamethyl-cyclodecasiloxane	741.54	112.0583	1928	0.0964

[a] From anthropogenic origin. From the column itself (bleeding).
[b] The deuterated compound helps in calibrating the GC-MS system and correcting for variations in the response of the mass spectrometer.
[c] Most likely comes from human applications of pesticides.
[d] Identified in the work of Ondeko et al., 2020, in the GC-MS results of *C. asiatica* methanol leaf extract [41].
[e] 2,4-bis[(trimethylsilyl)oxy]benzoic acid trimethylsilyl ester, often referred to as 2,4-bis(trimethylsilyl)oxybenzoic acid trimethylsilyl ester, is a silylated derivative of benzoic acid used in GC-MS analysis to enhance volatility and thermal stability of benzoic acid derivatives.
[f] Likely due to contamination or artifacts rather than a natural compound in the plants.

Table 4. GC-MS analysis of Launaea arborescens *essential oils.*

No.	CAS	Name of compound	Molecular weight (g/mol)	RT (min)	Kovats index	Area %
1	66-25-1	Hexanal	100.16	2.3872	900	0.0401
2	33746-69-9	cis-salvene	124.22	3.3172	940	0.0859
3	111-71-7	Heptanal	114.18	4.777	1002	0.0355
4	99-83-2	α-phellandrene	136.24	5.5834	1032	0.1818
5	5989-27-5	(+)-(4R)-limonene	136.24	5.7894	1039	0.1291
6	79-92-5	Camphene	136.24	6.4251	1063	0.2423
7	3387-41-5	Sabinene	136.23	7.9673	1219	0.4769
8	110-93-0	3-methyl-5-hepten-2-one	122.00	9.0856	1259	0.3258
9	127-91-3	Pinene	136.24	9.4682	1273	0.1243
10	554-61-0	2-carene	136.00	9.8038	1285	2.9893
11	99-83-2	l-phellandrene	136.24	9.998	1292	0.4948
12	99-86-5	α-terpinene	136.23	10.8397	1204	0.5947
13	138-86-3	Limonene	136.24	11.8109	1211	3.6812
14	7785-26-4	(-)-α-pinene	136.23	12.8116	1218	0.502
15	3779-61-1	(E)-β-ocimene	136.24	13.4826	1223	0.344
16	99-85-4	γ-terpinene	136.23	13.9064	1226	0.7628
17	15826-82-1	cis-sabinene hydrate	154.25	15.1366	1234	0.2499
18	586-62-9	α-terpinolene	136.23	15.8959	1239	0.2482
19	471-15-8	β-thujone	152.24	17.4499	1250	4.7275
20	586-62-9	α-terpinolene	136.23	18.1032	1255	1.9015
21	78-70-6	Linalool	154.25	18.5741	1258	6.7788
22	29803-81-4	trans-para-2-menthen-1-ol	154.25	19.616	1265	6.011
23	76-22-2	Camphor	152.23	20.0692	1268	1.9734
24	586-82-3	1-terpineol	154.25	20.9344	1274	3.8549
25	3208-16-0	2-ethylfuran	96.13	21.2994	1277	0.2661
26	10385-78-1	Borneol	154.25	22.4648	1285	0.1212
27	562-74-3	Terpinen-4-ol	154.25	22.8886	1288	2.0465
28	554-61-0	2-carene	136.23	24.3896	1298	2.843
29	16721-38-3	cis-piperitol	154.25	24.5309	1299	1.4929
30	562-74-3	Terpinene-4-ol	154.00	25.7434	1317	2.3312
31	15932-80-6	D-pulegone	152.23	26.7146	1331	0.2656
32	106-25-2	cis-geraniol	154.23	27.215	1338	0.4462
33	89-81-6	(±)-piperitone	152.23	27.7918	1347	0.294
34	106-24-1	Geraniol	154.25	29.3457	1369	1.5038
35	554-61-0	2-carene	136.00	34.1135	1442	0.1601
36	23726-93-4	β-damascenone	190.29	36.2148	1475	0.086
37	105-90-8	Geranyl propionate	210.32	36.7917	1484	0.0687

(*continued on next page*)

Table 4. (continued)

No.	CAS	Name of compound	Molecular weight (g/mol)	RT (min)	Kovats index	Area %
38	127-91-3	β-pinene	136.24	37.6334	1497	0.0956
39	17699-05-7	α-bergamotene	204.36	39.1344	1521	0.0637
40	19780-12-2	5-dodecyne	166.31	41.8479	1566	0.3248
41	1000273-87-2	3-(4-methoxyanilino)-1-methyl-pyrrolidine-2,5-dione	220.00	42.4718	1576	2.3052
42	13360-61-7	Pentadecene	210.40	43.084	1586	0.1201
43	17699-05-7	2,6-dimethyl-6-(4-methyl-3-pentenyl) bicyclo[3.1.1]hept-2-ene	204.35	43.9433	1601	0.516
44	483-76-1	delta-cadinene	204.36	44.3142	1607	0.1452
45	26560-14-5	(Z,E)-α-farnesene	204.35	45.7563	1632	0.2817
46	502-61-4	α-farnesene	204.36	46.5921	1647	0.3367
47	43219-68-7	1,4-dimethylcyclohex-3-enyl methyl ketone	171.50	47.1042	1656	0.7472
48	4602-84-0	Farnesol	222.37	48.2402	1676	13.5546
49	502-61-4	α-farnesene	204.36	48.511	1680	0.4304
50	23515-88-0	α-amorphene	204.35	49.1526	1692	0.3816
51	17699-14-8	α-cubebene	204.35	50.165	1710	0.7029
52	056348-21-1	Tricyclo[4.1.0.0(2,4)]heptane, 3,3,7,7-tetramethyl-5-(2-methyl-1-propenyl)	204.36	50.8124	1722	3.2444
53	473-15-4	2-[(2*R*,4*aR*,8*aS*)-4*a*-methyl-8-methylidene-1,2,3,4,5,6,7,8*a*-octahydronaphthalen-2-yl]propan-2-ol	222.37	52.6313	1755	22.3979
54	489-39-4	(+)-aromadendrene	204.36	52.9668	1761	0.3707
55	56599-94-1	1-bromo-8-heptadecyne	315.34	53.2905	1767	0.9038
56	502-61-4	α-farnesene	204.35	54.1617	1783	1.2103
57	2345-28-0	2-pentadecanone	226.39	54.8974	1797	0.4575
58	84348-07-2	(5*Z*)-trideca-1,5-diene	156.00	55.6508	1811	0.4037
59	17334-55-3	(+)-calarene	204.36	58.376	1864	0.6445
60	929625-08-1	2-(2,2,7,7-tetramethyltricyclo [6.2.1.01,6]undec-5-en-5-yl)propan-1-ol	202.33	62.1609	1939	0.2307
61	765-46-8	spiro[2.4]hepta-4,6-diene	92.00	62.9732	1956	0.4833
[a]62	2855-19-8	1,2-epoxydodecane	184.32	63.8385	1973	0.2509
63	694-92-8	2-methylnorbornene	108.18	64.3918	1984	0.2516
64	629-66-3	2-nonadecanone	282.50	65.0216	1997	0.3289
65	150-86-7	Phytol	296.53	74.8455	1985	0.1355

[a] Identified in the work of Ralte et al., 2022 [42], in the GC-MS results of *Parkia timoriana* extract and its medicinal use as an antimicrobial.

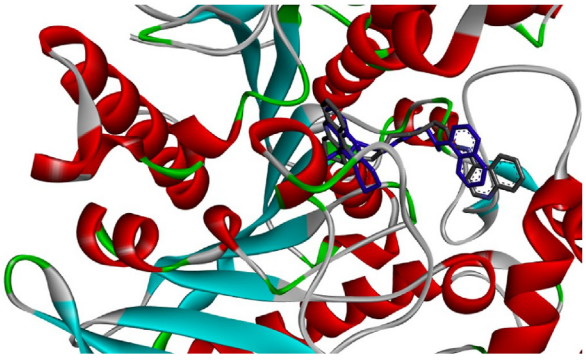


Fig. 5. Solid ribbon representation of the Tetronarce californica acetylcholinesterase enzyme (PDB ID: 1ODC) with cocrystal (gray) and redocked (blue) tacrine(8)-4-aminoquinoline.

Figs. 6 and 7 show that the reference ligand forms hydrogen bonds with Tyr121 and aromatic stacking interactions with Trp279, Phe330, Trp84, and Tyr70.

Table 5. The lowest binding energies (in kcal/mol) of the analyzed compounds are from Bubonium graveolens.

#	Compound	Lowest Binding Energy (Kcal/mol)
1	N-benzyl-N-ethyl-p-isopropylbenzamide	−9.6
2	Bicyclo[4.4.0]dec-1-ene, 2-isopropyl-5-methyl-9-methylene	−9.4
3	Naphthalene,1,2,3,4,4a, 7-hexahydro-1,6-dimethyl-4-(1-methylethyl)	−9.3
	Tacrine(8)-4-aminoquinoline (reference)	−11.0

N-Benzyl-N-ethyl-p-isopropylbenzamide also forms hydrogen bonds with Tyr121 and aromatic stacking interactions with several phenylalanine and tryptophan residues. Interestingly, the *B. graveolens* compounds lacking hydrogen bonds (bicyclo[4.4.0]dec-1-

Table 6. The lowest binding energies (in kcal/mol) of the analyzed compounds from Launaea arborescens.

#	Compound	Lowest Binding Energy (Kcal/mol)
1	Delta-cadinene	−9.6
2	Alpha-Cubebene	−9.1
3	alpha amorphene	−9
	Tacrine(8)-4-aminoquinoline (reference)	−11.0

ene and naphthalene) still exhibit good binding affinities through aromatic stacking and hydrophobic interactions. The *L. arborescens* compounds primarily rely on hydrophobic interactions with various residues, including His440, Tyr121, Tyr334, Phe330, and Trp432.

These docking data suggest that both *B. graveolens* and *L. arborescens* plants contain promising AChE inhibitors with diverse binding modes. While the

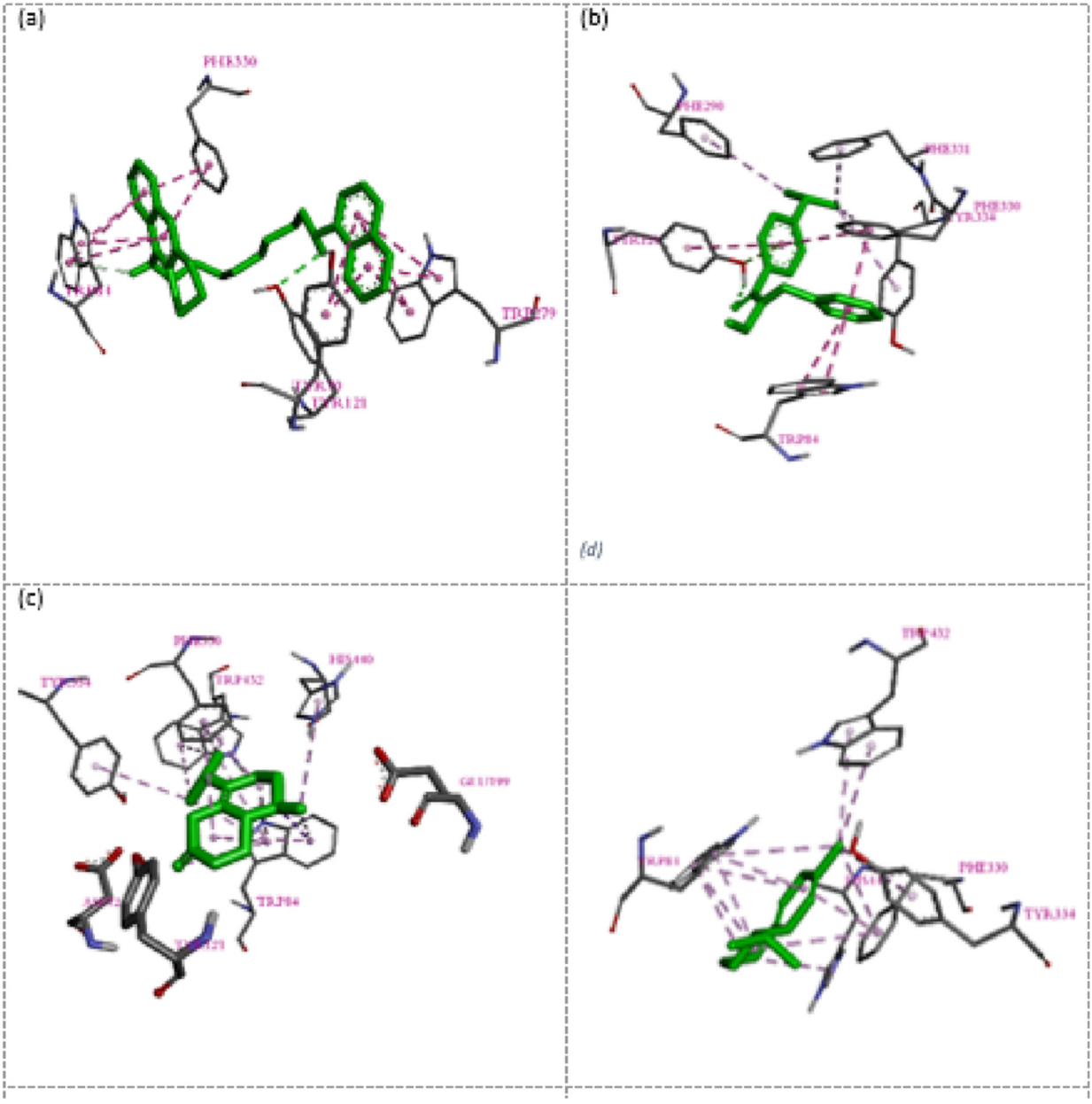


Fig. 6. Stick representation of (a) tacrine(8)-4-aminoquinoline (reference), (b) N-benzyl-N-ethyl-p-isopropylbenzamide, (c) bicyclo[4.4.0]dec-1-ene, 2-isopropyl-5-methyl-9-methylene, and (d) naphthalne,1,2,3,4,4a,7-hexahydro-1,6-dimethyl-4-(1-methylethyl), docked within the Tetronarce californica acetylcholinesterase enzyme (PDB ID: 1ODC) binding site.

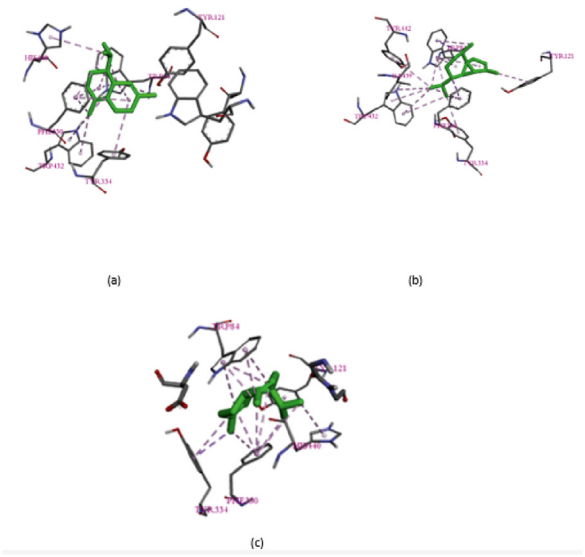


Fig. 7. Stick representation of (a) delta-cadinene, (b) alpha-cubebene, and (c) alpha amorphene, docked within the Tetronarce californica acetylcholinesterase enzyme (PDB ID: 1ODC) binding site.

reference ligand exhibited the strongest binding through hydrogen bonds and aromatic stacking, the *B. graveolens* compounds achieved good affinities through alternative interactions. Despite the presence of weak hydrogen bonds, the *L. arborescens* compounds potentially react through hydrophobic interactions. Overall, the docking results suggest that both *B. graveolens* and *L. arborescens* plants contain promising AChE inhibitors with diverse binding modes.

4. Conclusions

Several plant species can fight parasitic nematodes through the use of bioactive metabolites. The oil extracts obtained from the Arian region of *B. graveolens* and *L. arborescens* caused high mortality, reaching 78.56% and 85.71%, respectively, after 72 h. The above results demonstrate that the *L. arborescens* and *B. graveolens* oil extracts are potent nematicides. The toxicity of the oil extracts tested in this study may be due to the inhibition of the hatching process of egg masses by the absorption of bioactive compounds. The different types of nematicidal activity should be evaluated in other works to identify the species of *G. rostochiensis* cysts used in this work. The management of cyst nematodes by natural substances of plant origin is a process that quantitatively remains very limited. Molecular docking screening of the investigated compounds was performed to elucidate the molecular mechanisms underlying the hatching of cyst nematode (*G. rostochiensis* sp.) eggs from the aromatic herbs *B. graveolens* and *L. arborescens* on the acetylcholinesterase enzyme. Overall, the docking results indicate that *B. graveolens* and *L. arborescens* plants possess promising AChE inhibitors with a variety of binding mechanisms.

Ethics information

None.

Funding

Fund ID: B00L01UN1301201800.

Acknowledgments

The authors are thankful to the Algerian Ministry of Higher Education and Scientific Research and DGRSDT for the PRFU project (B00L01 UN1301201800).

References

[1] K. Fyad, N. Belboukhari, A.O. Hadj-Khelil, K. Sekkoum, Analgesic and anti-inflammatory activity of aqueous extract of *Bubonium graveolens*, Biomed Res Ther 7 (2020) 4002–4009, https://doi.org/10.15419/bmrat.v7i9.632.

[2] L.S. Seddiki, N. Belboukhari, A.O. El Hadj-Khelil, M.R. Sulaiman, K. Sekkoum, A. Cheriti, Pharmacological studies on aqueous extract of Launaea arborescens from southwest Algeria, J Ethnopharmacol 275 (2021) 114137, https://doi.org/10.1016/j.jep.2021.114137.

[3] S. Bhattarai, P.P.J. Haydock, M.A. Back, M.C. Hare, W.T. Lankford, Interactions between the potato cyst nematodes, Globodera pallida, G. rostochiensis, and soil-borne fungus, Rhizoctonia solani (AG_3), diseases of potatoes in the glasshouse and the field, Nematology 11 (2009) 631–640. https://brill.com/view/journals/nemy/11/4/article-p631_12.xml.

[4] J.W. Seinhorst, Effects of nematode attack on the growth and yield of crop plants, in: F. Lamberti, C.E. Taylor, eds., Cyst Nematodes. Nato ASI Series, vol. 121, Springer, Boston, MA. 1986, pp. 191–209, https://doi.org/10.1007/978-1-4613-2251-1_11.

[5] J.M.S. Faria, C. Vicente, Essential oils and volatiles as nematodicides against the cyst nematodes globodera and Heterodera, Biol Life Sci Forum 3 (2021) 1, https://doi.org/10.3390/IECAG2021-09689.

[6] V. Oro, S. Krnjajic, M. Tabakovic, J.S. Stanojevic, S. Ilic-Stojanovic′, Nematicidal activity of essential oils on a psychrophilic *Panagrolaimus* sp. (Nematoda: Panagrolaimidae), Plants 9 (2020) 1588, https://doi.org/10.3390/plants9111588.

[7] M.K. Stefanakis, C. Papaioannou, V. Lianopoulou, E. Philotheou-Panou, A.E. Giannakoula, D.M. Lazari, Seasonal variation of aromatic plants under cultivation conditions, Plants 11 (2022) 2083, https://doi.org/10.3390/plants11162083.

[8] Y. Oka, S. Nacar, E. Putievsky, U. Ravid, Z. Yaniv, Y. Spiegel, Nematicidal activity of essential oils and their components against the root-knot nematode, Phytopathology 90 (2000) 710–715, https://doi.org/10.1094/PHYTO.2000.90.7.710.

[9] P. Avato, S. Laquale, M.P. Argentieri, A. Lamiri, V. Radicci, T. D'Addabbo, Nematicidal activity of essential oils from aromatic plants of Morocco, J Pest Sci 90 (2017) 711–722, https://doi.org/10.1007/s10340-016-0805-0.

[10] S.K. Ibrahim, A.F. Traboulsi, S. El-Haj, Effect of essential oils and plant extracts on hatching, migration and mortality of

Meloidogyne incognita, Phytopathol Mediterr 45 (2006) 238–246. http://www.jstor.org/stable/26463259.
[11] E. Degroote, C. Schoorens, S. Pockelé, B. Stojilković, K. Demeestere, S. Mangelinckx, T. Kyndt, A combination of plant-based compounds and extracts acts nematicidal and induces resistance against *Meloidogyne incognita* in tomato, Front Plant Sci 15 (2024) 1411825, https://doi.org/10.3389/fpls.2024.1411825.
[12] F.J.C. Moreira, B. de A. Araújo, F.G. do N. Lopes, A. de A.L. de Sousa, A.E.C. Sousa, L.B. da S. Andrade, A.F. Uchoa, Assessment of the Tephrosia toxicaria essential oil on hatching and mortality of eggs and second-stage juvenile (J_2) root-knot nematode (*Meloidogyne enterolobii* and *M. javanica*), Aust J Crop Sci 12 (2018) 1829–1836, https://doi.org/10.21475/ajcs.18.12.12.p1102.
[13] A. Wahab, M. Muhammad, A. Munir, G. Abdi, W. Zaman, A. Ayaz, C. Khizar, S.P.P. Reddy, Role of arbuscular mycorrhizal fungi in regulating growth, enhancing productivity, and potentially influencing ecosystems under abiotic and biotic stresses, Plants 12 (2023) 3102, https://doi.org/10.3390/plants12173102.
[14] M.A. Ayub, G. Goksen, A. Fatima, M. Zubair, M.A. Abid, M. Starowicz, Comparison of conventional extraction techniques with superheated steam distillation on chemical characterization and biological activities of *Syzygium aromaticum* L. Essential oil, Separations 10 (2023) 27, https://doi.org/10.3390/separations10010027.
[15] Y. Murti, D. Jain, B.C. Semwal, S. Singh, P. Janmeda, P. Bhaskar, Innovative methods for extraction of essential oils from medicinal plants, Int J Second Metab 10 (2023) 190–230, https://doi.org/10.21448/ijsm.1121860.
[16] D. Kalaiselvi, A. Mohankumar, G. Shanmugam, G. Thiruppathi, S. Nivitha, P. Sundararaj, Altitude-related changes in the phytochemical profile of essential oils extracted from *Artemisia nilagirica* and their nematicidal activity against *Meloidogyne incognita*, Ind Crop Prod 139 (2019) 111472, https://doi.org/10.1016/j.indcrop.2019.111472.
[17] A. Dutta, A. Mandal, A. Kundu, M. Malik, A. Chaudhary, M.R. Khan, V. Shanmugam, U. Rao, S. Saha, N. Patanjali, R. Kumar, A. Kumar, S. Dash, P.K. Singh, A. Singh, Deciphering the behavioral response of *Meloidogyne incognita* and *Fusarium oxysporum* toward mustard essential oil, Front Plant Sci 12 (2021) 714730, https://doi.org/10.3389/fpls.2021.714730.
[18] I.N. Jardim, D.F. Oliveira, G.H. Silva, V.P. Campos, P.E. de Souza, P. E, (E)-Cinnamaldehyde from the Essential Oil of *Cinnamomum cassia* controls *Meloidogyne incognita* in soybean plants, J Pest Sci 91 (2018) 479–487, https://doi.org/10.1007/s10340-017-0850-3.
[19] L. Catani, B. Manachini, E. Grassi, L. Guidi, F. Semprucci, Essential oils as nematicides in plant protection—a review, Plants 12 (2023) 1418, https://doi.org/10.3390/plants12061418.
[20] K. Sekkoum, N. Belboukhari, A. Cheriti, New flavonoids from bioactive extract of algerian medicinal plant launeae arborescens, Asian Pac J Trop Biomed 4 (2014) 267–271, https://doi.org/10.12980/APJTB.4.2014C708.
[21] M.E. Said, I. Bombarda, J.V. Naubron, P. Vanloot, M. Jean, A. Cheriti, N. Dupuy, C. Roussel, Isolation of the major chiral compounds from Bubonium graveolens essential oil by HPLC and absolute configuration determination by VCD, Chirality 29 (2017) 70–79, https://doi.org/10.1002/chir.22672.
[22] Z. Souad, R. Linda, C. Abdelkrim, Effect of some saharan asteracea extrats (Launaea arboresens & Warionia saharae) against cyst nematode (Globodera Sp), PhytoChem BioSub J 8 (2014) 117–121. https://www.asjp.cerist.dz/en/article/43926.
[23] M.M.M. Abd-Elgawad, Optimizing safe approaches to manage plant-parasitic nematodes, Plants 10 (2021) 1911, https://doi.org/10.3390/plants10091911.
[24] S. Rodrigues, F.A.N. Fernandes, Extraction processes assisted by ultrasound, in: D. Bermudez-Aguirre, eds., Ultrasound: Advances for Food Processing and Preservation, Elsevier. 2017, pp. 351–368, https://doi.org/10.1016/b978-0-12-804581-7.00014-2.
[25] R.C. Hale, M.E. Seeley, A.E. King, L.H. Yu, Analytical chemistry of plastic debris: sampling, methods, and instrumentation, in: M.S. Bank, eds., Microplastic in the Environment: Pattern and Process, Springer International Publishing, Cham. 2022, pp. 17–67, https://doi.org/10.1007/978-3-030-78627-4_2.
[26] M. Adam, A. Westphal, J. Hallmann, H. Heuer, Specific microbial attachment to root knot nematodes in suppressive soil, Appl Environ Microbiol 80 (2014) 2679–2686, https://doi.org/10.1128/AEM.03905-13.
[27] S.J. Turner, K. Evans, The origins, global distribution and biology of potato cyst nematodes (Globodera rostochiensis (Woll.) and Globodera pallida Stone), in: R.J. Marks, B.B. Brodie, eds., IPotato Cyst Nematodes: Biology, Distribution and Control, CABI International, Wallingford, Oxon (CABI). 1998, pp. 7–26. https://repository.rothamsted.ac.uk/item/884y7/the-origins-global-distribution-and-biology-of-potato-cyst-nematodes-globodera-rostochiensis-woll-and-globodera-pallida-stone.
[28] M. Senthilkumar, N. Amaresan, A. Sankaranarayanan, Extraction of nematodes from plant materials, in: Plant-Microbe Interactions, Springer Protocols Handbooks. Humana, New York, NY. 2021, https://doi.org/10.1007/978-1-0716-1080-0_77.
[29] S. Sellami, T. Mezrket, T. Dahmane, Activite nematicide de quelques huiles essentielles contre *Meloidogyne incognita*, Nematol Medit 38 (2010) 195–201. https://journals.flvc.org/nemamedi/article/view/87037.
[30] V. Būda, R. Cepulytė-Rakauskienė, The effect of linalool on second-stage juveniles of the potato cyst nematodes Globodera rostochiensis and *G. pallida*, J Nematol 43 (2011) 149–151. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3547347/.
[31] J. Eberhardt, D. Santos-Martins, A.F. Tillack, S. Forli, AutoDock Vina 1.2.0: new docking methods, expanded force field, and Python bindings, J Chem Inf Model 61 (2021) 3891–3898, https://doi.org/10.1021/acs.jcim.1c00203.
[32] O. Trott, A.J. Olson, AutoDock Vina: improving the speed and accuracy of docking with a new scoring function, efficient optimization, and multithreading, J Comput Chem 31 (2010) 455–461. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3041641/.
[33] E.H. Rydberg, B. Brumshtein, H.M. Greenblatt, D.M. Wong, D. Shaya, L.D. Williams, P.R. Carlier, Y.-P. Pang, I. Silman, J.L. Sussman, Complexes of alkylene-linked tacrine dimers with torpedo californica acetylcholinesterase: binding of bis(5)-tacrine produces a dramatic rearrangement in the active-site gorge, J Med Chem 49 (2006) 5491–5500, https://doi.org/10.1021/jm060164b.
[34] K. Eloh, K. Kpegba, N. Sasanelli, H.K. Koumaglo, P. Caboni, Nematicidal activity of some essential plant oils from tropical West Africa, Int J Pest Manag 66 (2019) 131–141, https://doi.org/10.1080/09670874.2019.1576950.
[35] L.D.P. Ribeiro, M.S. Santos, G.L.P. Gonçalves, J.D. Vendramim, Toxicity of an acetogenin-based bioinsecticide against diaphorina citri (Hemiptera: liviidae) and its parasitoid *Tamarixia radiata* (hymenoptera: eulophidae), Fla Entomol 98 (2020) 835–842, https://doi.org/10.1653/024.098.0304.
[36] F. Khan, M. Asif, A. Khan, M. Tariq, T. Ansari, M. Shariq, M.A. Siddiqui, Evaluation of the nematicidal potential of some botanicals against root-knot nematode, Meloidogyne incognita infected carrot: in vitro and greenhouse study, Curr Plant Biol 20 (2019) 100115, https://doi.org/10.1016/j.cpb.2019.100115.
[37] N. Sasanelli, I. Toderas, P. Veronico, E. Iurcu-Straistaru, S. Rusu, M.T. Melillo, P. Caboni, Abamectin efficacy on the potato Cyst Nematode globodera pallida, Plants 9 (2019) 12, https://doi.org/10.3390/plants9010012.
[38] D.X. Amora, G.S. de Podesta, P.H.F. Grupioni, É. das Graças Carvalho Nasu, L.D. de Figueiredo, F.C. Ferreira, L.G. de Freitas, E.A. Lopes, S. Ferraz, Effect of essential oils on the root-knot nematode management, Agri-Env Sci AGRIES 3 (2017) 15–23, https://doi.org/10.36725/agries.v3i1.225.

[39] P. Barbosa, A.S. Lima, P. Vieira, L.S. Dias, M.T. Tinoco, J.G. Barroso, L.G. Pedro, A.C. Figueiredo, M. Mota, Nematicidal activity of essential oils and volatiles derived from Portuguese aromatic flora against the pinewood nematode, *Bursaphelenchus xylophilus*, J Nematol 42 (2010) 8–16. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3380513/.

[40] W. Hassan, S. Rehman, H. Noreen, S. Gul, Neelofar, N. Ali, Gas chromatography mass spectrometric (GCMS) analysis of essential oils of medicinal plants, Adv Anim Vet Sci 4 (2016) 420–437, https://doi.org/10.14737/jounal.aavs/2016/4.8.420.437.

[41] D.A. Ondeko, B.F. Juma, L.D. Baraza, P.K. Nyongesa, LC-ESI/MS and GC-MS methanol extract analysis, phytochemical and antimicrobial activity studies of Centella asiatica, Asian J Chem Sci 8 (2020) 32–51, https://doi.org/10.9734/AJOCS/2020/v8i319046.

[42] L. Ralte, L. Khiangte, N.M. Thangjam, A. Kumar, Y.T. Singh, GC-MS and molecular docking analyses of phytochemicals from the underutilized plant, Parkia timoriana revealed candidate anti-cancerous and anti-inflammatory agents, Sci Rep 12 (2022) 3395, https://doi.org/10.1038/s41598-022-07320-2.