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Acetylcholinesterase, Tyrosinase, α-Glucosidase inhibition of *Ammodaucus leucotrichus* Coss. & Dur. Fruits Essential oil and Ethanolic Extract and Molecular Docking Analysis

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Abstract: The medicinal and aromatic plants are a source of bioactive molecules and mineral compounds used for therapeutic and agro-food purpose. This study aimed at the evaluation of the inhibitory enzyme effect of *Ammodaucus leucotrichus* Coss & Dur fruits essential oil, aqueous and ethanol extract against acetylcholinesterase, tyrosinase and α-glucosidase, and the evaluation of the antioxidant activity of these natural mixtures using tree methods (DPPH, FRAP and β-carotene bleaching tests). Moreover, this study investigates the mineral composition of different parts of studded plant. The different natural mixtures studied show a significant inhibitory effect on Acetylcholinesterase (67.56-92.30%), Tyrosinase (57.52-63.44%) and α-Glucosidase (61.22-72,49%). The studied extracts also show an important antioxidant effect. In addition, the obtained results show the abundance of macro and microelements, like calcium (2.028 mg/g for leaves and 1.787 mg/g for fruits) in *Ammodaucus leucotrichus* Coss & Dur plant. The present study is in favor of the importance of the exploitation of *Ammodaucus leucotrichus* Coss & Dur fruits in the pharmaceutical and agro-alimentary fields. Molecular docking studies were employed to predict the therapeutic properties of Ammodaucus leucotrichus Coss & Dur fruits.

Keywords: *Ammodaucus leucotrichus;* minerals composition; essential oil; AChE; Tyrosinase; α-Glucosidase; Molecular Docking.

1. Introduction

The oxidative stress is recognized as the main factor in the occurrence of many health disorders such as Alzheimer disease (AD) that is a chronic neurological disorder that causes memory

problems, cognitive dysfunction, behavioral problems and an incapacitation in the daily routine. To reduce the risk of these diseases, the researchers found that an increasing amount of acetylcholine by AChE enzyme inhibitor is the most treatment strategy of AD (Takim *et al.,* 2021). Unfortunately, the current therapeutic drugs used as AChE enzyme inhibitor have been reported to have several side effects like the hepatotoxicity, gastrointestinal disturbances and cardiovascular problems (Aktumsek et al., 2013; Işık & Beydemir, 2021). Moreover, an increased level of oxidative stress in cell skin contributes to the activation of melanogenesis by producing reactive oxygen species by activating tyrosinase enzyme. That leads to various skin hyperpigmentation disorders such as melasma, seborrheic keratoses, melasmas and malignant melanomas, diabetic dermopathy and tinea versicolor (Chang *et al.,* 2013). Additionally, tyrosinase is thought to be the cause of neuromelanin production and neuronal damage associated with Parkinson's disease (Asanuma *et al.,* 2003). Unfortunately, the synthetic or microbial tyrosinase inhibitors widely used to combat this phenomenon are not stable, such as hydroquinone, Arbutin and Kojic acid (Zhao *et al.,* 2021). Indeed, the abundant use of these compounds can lead to skin cancer and other diseases. Furthermore, there is also a relationship between oxidative stress and diabetes mellitus type 2. The high levels of cellular glucose increase the production of reactive oxygen species (ROS) and the oxidative stress may directly promote the occurrence of diabetes mellitus type 2 by decreasing insulin sensitivity and destroying the insulin-producing cells within the pancreas (Yang *et al.,* 2011). Thus, research for an alternative to traditional antioxidant agents and enzyme inhibitors, known for their negative effect, has been developed. Those researches assures that natural mixtures isolated from aromatic and medicinal plants show significant enzymes inhibition and antioxidant effect with minor safety risks (Dandlen *et al.,* 2011; Najibullah *et al.,* 2021; Ouknin *et al.,* 2018). These behaviors of natural mixtures extracted from medicinal and aromatic plants have been attributed to their richness in chemical compounds especially phenolic compounds, that show an important activity against enzymes (Ouknin *et al.,* 2021). These effects encourage researchers to characterize the secondary metabolites profile of this type of plants, that representing also a source of minerals with high nutritional value that could prevent individual risk factors for certain diseases (Bhat *et al.,* 2010; Sanchez-Castillo *et al.,* 1998).

The *Ammodaucus leucotrichus* (AML) is an annual medicinal plant belonging to *Apiaceae* family growing generally in North Africa in the grazing. In North Africa, the fruits of this plant are traditionally used to flavor tea. Those fruits are used in traditional medicine such as a condiment and a treatment of colds, fever and digestive disorders for children (Idm'hand *et al.,* 2020). In addition, the essential oil of *Amomoducus leucotrichus* aerial part exhibits antimicrobial and antioxidant activities (Manssouri *et al.,* 2016; Louail *et al.,* 2016; Dahmane *et al.,* 2017). The richness of AML oil in various chemical compounds was used as corrosion inhibitor of tinplate in 0.5M $H_2C_2O_4$ (Boumezzourh *et al.,* 2019).

Recently, we also reported that essential oil and aqueous extrats of *Ammodaucus leucotrichus* exhibited higher antioxidant activity. We showed that a positive correlation was observed between antioxidant activity and the total phenolic and flafonoid contents of aqueous extrats studied (Manssouri *et al.,* 2020). The importance of the antioxydatnt activity we observed in this study led us to investigate the possibility of exploiting secondary metabolites from *Ammodaucus leucotrichus* in reducing the effect of oxidative stress diseases. Thus, in this article, we are particularly interested in the evaluation of inhibitory enzymes such as AChE and mainly tyrosinase and a-glucosidase in ethanolic and aqueous extracts, and essential oils of *Ammodaucus leucotrichus* fruits. The mineral composition of these fruits was also established using inductively coupled plasma mass spectrometry.

2. Methodology

2.1 Plant material

The *Ammodaucus leucotrichus* (Apiaceae family) was harvested on May 2020 in Boudenib/South-East Morocco (31°56'59N, 3°35'28W). The plant was identified following practical flora of Morocco (Fennane *et al.*, 1999) and preserved in the herbarium of Science and Techniques Faculty of Errachidia (ER-20-10). The plant's fruits and leaves were dried in the dark at room temperature, then separated before being ground.

2.3 Essential oil isolation and GC–MS analysis

The essential oil studied was isolated and characterized as described in our previous research work (Boumezzourh *et al.*, 2019).

2.4 Extract preparation

The aqueous and ethanol extracts were prepared using the maceration technique. Each 10g sample of AML fruits powder was mixed with 50 mL of distilled water or pure ethanol. The suspension obtained was stirred for 1h then macerated for 24 hours at room temperature. After filtration of extract, the solvent was evaporated.

2.5 Enzyme inhibitory test

2.5.1 AChE inhibition

The Cholinesterase inhibitory activity of AML extracts was evaluated using a microplate reader as described by Ellman *et al.*, (1961) with a little modification. The essay was initiated by mixing 25 µL of 15 mM ATCI with 125 µL of 3 mM DTNB. Then 50 µL of 100 mM phosphate buffer (pH 8.0) and 25 µL of each essential oil /extract at different concentrations 0.25, 0.5, 0.75 and 1 mg/mL were added. For positive and negative control, 25 µL of galantamine or buffer were used respectively. Before measuring the absorbance at 405 nm for 5 min, 0.28 U/mL AChE was added to the obtained mixtures. The test was performed in triplicate.

2.5.2 Tyrosinase inhibition

The inhibitory activity of AML against enzyme tyrosinase was evaluated using the Spectrophotometry according to the method reported by Masuda *et al.*, (2005). To that end, 0.4 mg/mL of each sample (extracts or essential oil) at different concentrations ranging between 0.25 and 1 mg/mL were mixed with 80 µL of phosphate buffer (pH 6.8), 40 µL of L-DOPA and 40 µL of tyrosinase. Phosphate buffer and Kojic acid (200 µg/mL) were used as blank and reference, respectively. The inhibition activity is given in percentage of inhibition (%) after measuring the absorbance of the mixture at 475nm.

2.5.3 α-Glucosidase inhibition

The evaluation of α-glucosidase inhibition was carried as described by Kwon *et al.*, (2008). 50 µL of each sample (AML extracts or essential oil) at different concentrations ranging from 0.25 to 1 mg/mL, or 1 mg/mL of acarbose (positive control: an anti-diabetic drug used to treat diabetes mellitus type 2 were mixed with 100 µL of 0.1M phosphate buffer (pH 6.9) containing yeast α-glucosidase (1.0 U/mL). The obtained solution was incubated at room temperature for 10 min, and then 50 µL of p-nitrophenyl-α-D-glucopyranoside solution (5 mM) were added. After another 10 min incubation, the absorbance was evaluated at 405 nm. The α-glucosidase inhibitory activity was calculated as percent inhibition. All tests were performed in triplicate.

2.6 Mineral composition analysis

After grinding the dry fruits and leaves of AML, each 0.5g of obtained powders was digested in 2ml of sulfuric acid, 6ml of nitric acid and 6ml of oxygenated water (H_2O_2). After heating the mixture for 30 minutes, the mineral deposit was cooled down then filtered. The obtained filtrate was adjusted to 25mL with 0.1M HNO_3. To prevent contamination, all procedures of handling were conducted without metal contact. The determination of minerals in the obtained solution was performed using inductively coupled plasma mass spectrometry (Jobin-Yvon 7O ICP) ULTIMA AND JY70.

2.7 Statistical Analysis

SPSS 25 for Windows (SPSS Inc., Chicago, IL, USA), was used to conduct the statistical analysis. Descriptive analysis of the data, including mean, standard deviation (S.D), was performed. Tukey's test ($P \leq 0.05$) was also used to compare the means of all concentrations and each enzyme.

2.8. Preparation of ligands

The selection encompassed the main constituents within the volatile fraction of Ammodaucus leucotrichus fruits, which were pre-concentrated using Headspace Solid Phase Microextraction (HS-SPME). These constituents were chosen due to their potential therapeutic and agro-food-related properties. The source of these compounds was the fruits of Ammodaucus leucotrichus Coss & Dur, commonly utilized in herbal remedies. Their structural data was procured from the PubChem database (http://pubchem.ncbi.nlm.nih.gov) in the form of Structure Data File Format (SDF) (Bourhou *et al.*, 2023). The three-dimensional structures (3D) of these compounds, including the control ligand Alpha-Tocopherol **Table 4**,were meticulously prepared to facilitate molecular docking investigations. Employing a suite of controlled algorithms within Maestro 12.8, 3D and geometric optimizations were conducted, coupled with ligand energy minimization (Diass *et al.*, 2023a). Hydrogen atoms were introduced, salt components were removed, and ionization was executed at pH 7 ± 2, employing the LigPrep module. The energy minimization process was executed through the utilization of the OPLS4 force field.

2.9. Protein preparation and Molecular docking calculations

Molecular docking studies were performed for Acetylcholinesterase, Tyrosinase, and α-Glucosidase using the X-ray crystal structures represented by (PDBID: 1C2B), (PDBID: 2Y9W), and (PDBID: 3WY1), respectively. The protein structures were meticulously prepared through the utilization of the Protein Preparation Wizard (Maestro 12.8) (Cherriet *et al.*, 2023). This involved the removal of ligand and water atoms, followed by the merging of non-polar hydrogen atoms. The grid box coordinates were set at x=20 Å, y=20 Å, and z=20 Å, with the incorporation of the extra Precision (XP) glide score for predicting binding free energy, ligand strain energy, and the selection of docked conformations. Docking scores were then presented as affinity binding values (Kcal/mol). The energy minimization step involved the application of the OPLS4 force field, utilizing a default RMSD limit of 0.3 Å. Ultimately, the protein's structure underwent minimization, resulting in the selection of the conformation featuring the lowest binding energy (Fajriyah, *et al.*, 2023). The conformation characterized by the lowest binding energy was chosen as the optimal final structure. This structure was depicted through both two-dimensional and three-dimensional diagrams, and the analysis and visualization were carried out using BIOVIA Discovery Studio, 2021.

3. Results and Discussion

3.1 Enzyme inhibitory activities

Ammodaucus leucotrichus fruits essential oil and fruits extracts were tested for the first time for their effect against AChE, Tyrosinase and α-Glucosidase enzymes. From **Table 1**, it clearly emerges that the essential oil and the extracts show an inhibitory effect against the three enzymes studied. This effect depends on the concentration and the nature of the natural complex mixtures tested.

Table 1. Enzyme inhibitory activity: AChE, Tyrosinase and α-Glucosidase.

	Concentration	AChE (%)	Tyrosinase (%)	α-Glucosidase (%)
Essential oil	0.25 mg/mL	47.85±0.15d	36.22±0.13d	39.80±0.11d
	0.5 mg/mL	64.93±0.37g	40.85±0.22f	47.71±0.33f
	0.75 mg/mL	78.07±0.10j	50.62±0.27h	58.64±0.25h
	1 mg/mL	92.32±0.05l	63.60±0.08k	72.49±0.20k
Aqueous extract	0.25 mg/mL	34.78±0.21a	29.06±0.39a	30.76±0.07a
	0.5 mg/mL	40.63±+0.09b	33.44±0.10c	37.05±0.18c
	0.75 mg/mL	50.47±0.08e	45.80±0.10g	47.64±0.12f
	1 mg/mL	67.56±0.18h	59.78±0.26j	61.22±0.07i
Ethanol extract	0.25 mg/mL	43.51±0.07c	31.62±0.21b	34.42±0.11b
	0.5 mg/mL	58.62±0.07f	39.05±0.27e	43.70±0.12e
	0.75 mg/mL	64.71±0.13g	45.55±0.20g	54.86±0.21g
	1 mg/mL	83.77±0.11k	57.52±0.20i	65.47±0.10j
Positive control		75.04±0.28i	77.46±0.16l	88.50±0.23l

Values are expressed as mean ± SE (n = 3). In the same column, values marked with different letters indicate significant differences (P<0.05; Tukey test).

The AChE inhibitor efficacy of *Ammodaucus leucotrichus* fruits essential oil and extracts was compared with the effect of the galantamine as a positive control. **Table 1** shows that efficiency raises by increasing the concentration of the extract tested. It is also revealed that essential oil exhibits the highest inhibition efficiency even from a concentration of 0.75 mg/mL of oil. The inhibition efficiency (78.07%) is higher than that of the positive controls (75.04%). The most potent activity of 92.32% is obtained by essential oil at 1mg/mL followed by ethanolic extract with 83.77% at 1mg/mL. The inhibitory effect of AML oil and extracts can be attributed to their main compounds or to the synergy between these compounds. In order to identify the compounds responsible for AChE enzyme inhibition, a previous study compared the effect of AML essential oil and its main pure compounds, perillaldehyde and limonene. The cited study shows that the most potent activity was obtained for limonene (Sadaoui *et al.*, 2018).

From **Table 1**, the tyrosinase inhibition effect of essential oil and AML extracts show that the essential oil exhibits the highest tyrosinase inhibition activity with 63.60% at 1mg/mL, followed by aqueous extract (59.78%) and ethanolic extract (57.52%) at the same concentration. The high inhibition activity of essential oil can be attributed to the hydrophobic part of its constituents, which act as competitive inhibitors of tyrosinase enzyme (Taherkhani, 2016). While the tyrosinase inhibitory activity of AML extracts may be attributed to the interaction between, the active side of the enzyme and the hydroxyl groups of phenolic compounds extracts (Kooltheat *et al.* 2023; Navia *et al.* 2020; Li *et al.*, 2004). However, the inhibitory effect of the studied oil and the extracts remains lower than that of Kojic acid (77.47 % at 200µg/mL) used as positive control.

The inhibitory activity of essential oil, ethanolic and aqueous extracts of *Ammodaucus leucotrichus* fruits against α-glucosidase were evaluated for the first time, and the obtained results are presented in **Table 1**. The inhibition efficiency of the three natural mixtures studied depends on the concentrations and the nature of extract. The essential oil shows the high inhibition efficiency (72.49% at 1mg/mL) followed by ethanolic extract and then the aqueous extract (65.47 and 61.22 % respectively at 1mg/mL). However, at the same concentration of 1mg/mL the acarbose exhibits inhibition efficiency against the α-glucosidase of 88.10%. The high inhibitory effect of essential oil could be caused by the presence of limonene that is reported exhibiting high α-glucosidase inhibition (Sahin Basak and Candan, 2013), or the synergy between the main essential oil compounds and the other compounds. For the inhibitory effect of ethanolic extract and aqueous extract, it can be explained by their richness in phenolic compounds that are known for their ability to bind to proteins through hydrogen bonding. Similarly, Zengin *et al.*, (2016) report that total phenolics, flavonoids, and tannins contained from eight Centaurea species showed strong activity against cholinesterase, tyrosinase, α-amylase, and α-glucosidase.

3.2 Mineral composition

Mineral analysis (ICP-AES) of AML fruits and leaves, show significant variations in mineral element content among plant parts. The contents of the 23 mineral elements evaluated in the studied parts of AML are presented in **Table 2**.

Table 2. Mean concentration of minerals in *Ammodaucus leucotrichus* fruits and leaves (mg/g).

Element	Leaves		Fruits	
	Mean	S.D.	Mean	S.D.
Al	0.144	0.004	0.144	0.00219
As	<0.010	<0.010	<0.010	<0.010
B	0.059	0.01	0.058	0.008
Ba	0.06	0.01	0.057	0.0015
Bi	0.139	0.006	0.166	0.0037
Ca	2.028	0.008	1.787	0.015
Cd	<0.004	<0.004	<0.004	<0.004
Cr	0.067	0.009	0.066	0.0008
Cu	<0.003	<0.003	<0.003	<0.003
Fe	0.020	0.002	0.020	0.002
K	0.011	0.001	0.010	0.001
Li	0.030	0.003	0.030	0.001
Mg	1.375	0.006	1.374	0.014
Mn	<0.001	<0.001	<0.001	<0.001
Na	<0.108	<0.108	<0.108	<0.108
Ni	0.057	0.004	0.043	0.007
P	0.896	0.04	0.846	0.02
Pb	<0.011	<0.011	<0.011	<0.011
Sn	0.122	0.003	<0.015	<0.015
Sr	0.057	0.0016	0.057	0.0016
V	0.024	0.002	0.0435	0.002
Zn	<0.002	<0.002	<0.002	<0.002
Zr	0.044	0.0008	0.045	0.001

The results of ICP-AES analysis clearly show that *Ammodaucus leucotrichus* constitutes an interesting source of mineral elements (**Table 2**). Calcium (Ca) is the major macro-element detected in AML leaves (2.028 mg/g) and fruits (1.787 mg/g). It is followed by magnesium (Mg) at 1.375 mg/g in leaves and at 1.374 mg/g in fruits, then phosphorus (P) at 0.896 mg/g in leaves is 0.896 mg/g and at 0.846 mg/g in fruits. However, the sodium content is 0.108 mg/g for both samples and the potassium (K) was detected at a level less than 0.01 mg/g in the two studied parts of *Ammodaucus leucotrichus*.

Regarding the microelement, aluminum (Al) is present at 0.144 mg/g in fruits and leaves. AML fruits are rich in Bismuth (Bi) (0.166 mg/g) compared to leaves (0.139 mg/g). Silicon (Si) is present in the both studied parts of the plant at 0.136 mg/g. The tin (Sn) content in leaves is 0.122 mg/g whereas it is only 0.015 mg/g in fruits. Iron (Fe) is only present at 0.020 mg/g of the both tested parts of our plant. Copper (Cu) is only detected in trace amounts with a content of less than 0.003 mg/g in both powders.

According to the literature (Ziani *et al.*, 2019), AML is an excellent source of macro elements with Ca at 15.55 mg/g, K at 22.83 mg/g, Mg at 2.366 mg/g and Na at 1.60±0.06 mg/g in the areal parts. However, they found Fe and Cu concentrations almost similar to those obtained in our samples (Ziani *et al.*, 2019). Soil properties, the geographical diversity, growing conditions, time of harvest and genetic plant factors could be the causes of the differences found between our samples and others regarding mineral composition (Dueli *et al.*, 2021; Radha *et al.*, 2021).

The *Ammodaucus leucotrichus* plant could help to provide a part of daily minerals need of human body. Moreover, its low sodium (Na) content represents an advantage regarding to the relationship between sodium and hypertension (Okwu, 2005). The concentrations of Pb and Cd in our samples are under than 0.011 mg/g and 0.004 mg/g, respectively. The heavy metals content found to be below the recommended maximum acceptable levels proposed by the Joint FAO/WHO Expert Committee on Food Additives.

Table 3. Major elemental composition of the bios and hybrid bios

S/N	Element	Biomass Biochar		Hybrid Biochar	
		Atomic Conc.	**Weight Conc.**	**Atomic Conc.**	**Weight Conc.**
1	Carbon	7.13	57.9	86.9	75.46
2	Silicon	9.63	17.5	1.95	3. 59
3	Potassium	4.17	10.5	3.46	9.79
4	Oxygen	9.57	9.94	4.59	5.131
5	Nitrogen	0.85	0.78	1.26	1.127
6	Chlorine	0.38	0.89	0.50	1.219
7	Calcium	0.26	0.67	0.25	0.712
8	Aluminum	0.33	0.57	0.26	0.150
9	Phosphorus	0.26	0.52	0.26	0.528
10	Magnesium	0.26	0.40	0.28	0.520
11	Sulfur	0.12	0.24	0.19	0.424
12	Sodium	0.06	0.08	0.11	0.128

3.3. Molecular docking studies

The molecular docking technique serves as a valuable computational tool within the realm of chemistry. It facilitates the simulation and examination of interactions occurring at the atomic level between proteins and small molecules. Employing this approach, scientists acquire valuable insights into the manner in which small molecules behave within the binding regions of target proteins. Consequently, this method contributes to the progression of our comprehension pertaining to essential biochemical mechanisms (Diass *et al.*, 2023b; Merzouki *et al.*, 2023; Haddou *et al.*, 2023;) . The results obtained from molecular docking simulations involving phytochemicals and their interactions with Acetylcholinesterase, Tyrosinase, and α-Glucosidase have been presented in **Table 4.** The data clearly demonstrates that all compounds exhibited affinities elevated with the exception of Limonene compared to the α-Tocopherol control. Thymol exhibited the highest affinities towards the active sites of Acetylcholinesterase, Tyrosinase, and α-Glucosidase. Notably, Thymol's affinities were even superior to those of the positive control α-Tocopherol utilized in this study, yielding respective binding energies of -6.098, -3.254, and -5.210 kcal/mol. The binding energies associated with the interactions at the active sites of Acetylcholinesterase, Tyrosinase, and α-Glucosidase were determined to be -7.369 kcal/mol, -5.239 kcal/mol, and -5.350 kcal/mol, respectively. The docking molecular analyses were carried out with the aim of clarifying the interaction modes of the first compound exhibiting the highest affinity toward target receptors, thus explaining the mechanism of action performed by this phytochemical molecule. In general, the predominant interactions contributing to the formation of the complexes encompass Conventional Hydrogen Bonds, Pi -Alkyl Interactions, Alkyl bonds, Pi-Pi-Stacked and Van der Waals forces **Figure 1.** Thymol who showed the highest inhibition power towards the active site of the Acetylcholinesterase, has recruited several residues of amino acids through solid interactions essentially of the conventional hydrogen bond type (ARG296 and PHE295), Pi-Akyl (TRP286, TYR337, PHE338 and TYR341), Pi-Pi-Stacked (TRP286) and Van der Waals (SER293, TYR124, PHE297, LEU289, ILE294). The findings distinctly demonstrate the existence of bioactive compounds possessing notable inhibitory potential against the active sites of the proteins Acetylcholinesterase, Tyrosinase, and α-Glucosidase. Among all the phytochemical compounds examined, Thymol exhibited the highest binding energy values, signifying the most significant inhibitory activities. Notably, Thymol's inhibitory activities greatly surpassed those of the control compound. Further clinical and laboratory investigations are imperative to solidify the therapeutic potential of the primary constituents found in the volatile fraction of the essential oil extracted from Ammodaucus leucotrichus fruits. These investigations are crucial to fully comprehend the viability and efficacy of this essential oil for potential therapeutic applications.

Table 4. Docking Scores results of selected compounds against Acetylcholinesterase, Tyrosinase and α-Glucosidase.

Nº	Compound name	Docking Scores (kcal/mol)		
		Acetylcholinesterase	Tyrosinase	α-Glucosidase
1	Carvacrol	-6.838	-5.284	-4.882
2	E-Anéthol	-5.015	-5.284	-4.484
3	Limonène	-4.600	-4.028	-3.167
4	Périllaldéhyde	-7059	-4.186	-4.260
5	Thymol	-7.367	-5.239	-5.350
6	α-Tocopherol	-6.098	-3.254	-5.210

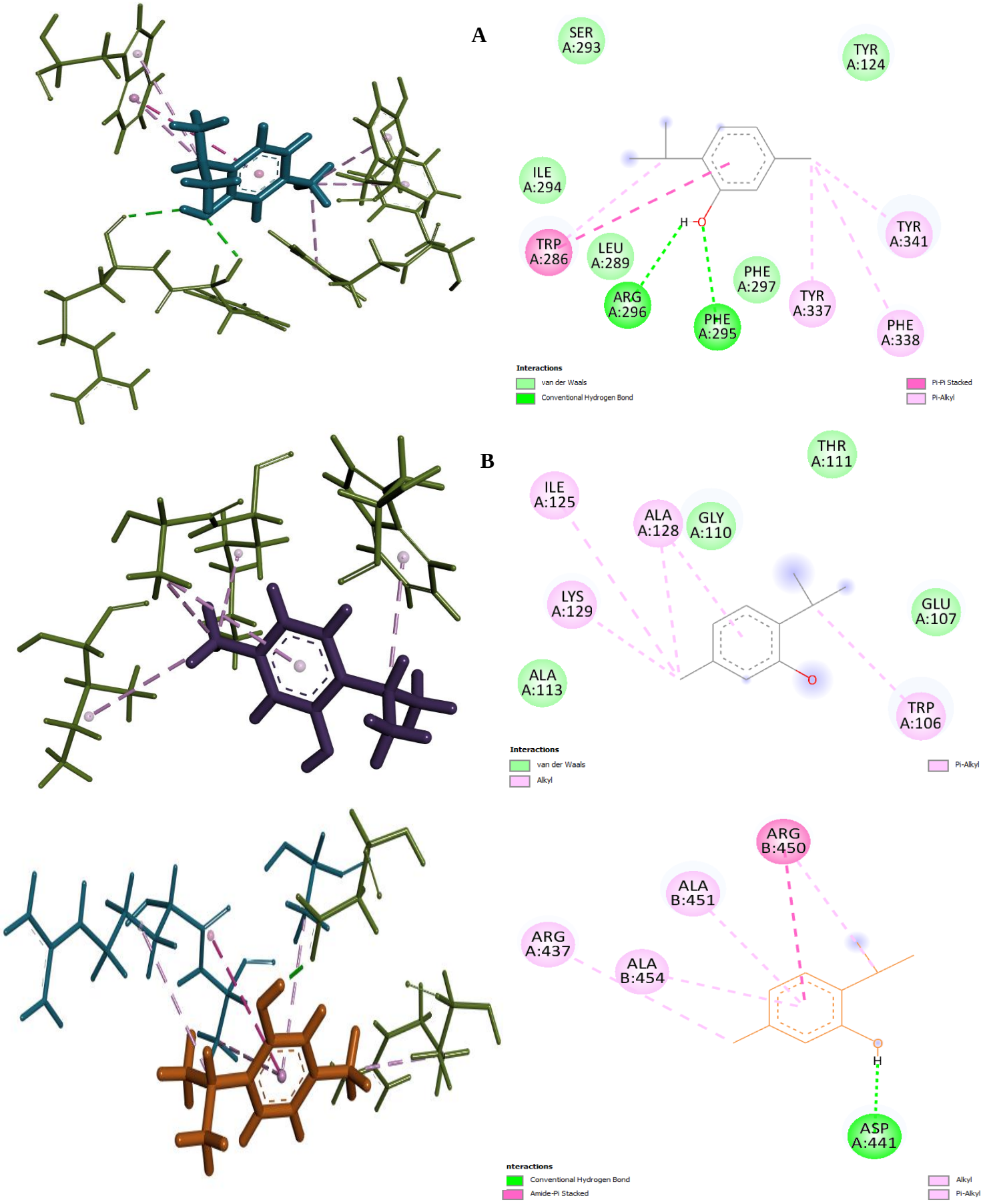

Figure.1. 2D and 3D-representations of the chemical bonding modes of the complexes formed between Thymol compound and the (A)Acetylcholinesterase, (B)Tyrosinase and (C) α-Glucosidase.

Conclusion

The essential oil, aqueous and ethanolic extracts *of Ammodaucus leucotrichus* Coss & Dur fruits show an inhibitory effect against AChE, Tyrosinase and α-Glucosidase enzymes. This allows us to say that the studied plant may be used to reduce the risk of Alzheimer's disease, diabetes mellitus type 2 and skin diseases. The ICP-AES analysis of the fruits and leaves of *Ammodaucus leucotrichus* shows that this plant is rich in macro and microelements. The highest content is detected for calcium 2.028 mg/g followed by Magnesium 1.375 mg/g. However, the element concentrations depend on the part of plant. From the obtained results, we can conclude that *Ammodaucus leucotrichus* Coss & Dur represents a source of mineral and bioactive compounds, which supports the possible use of this plant in the pharmaceutical and food industries. Molecular docking has demonstrated its cost-effective utility in identifying potential drug targets, thereby validating the therapeutic attributes of essential compounds present in Ammodaucus leucotrichus Coss & Dur fruits. Nonetheless, additional laboratory and clinical investigations are warranted to substantiate these findings.

Disclosure statement: *Conflict of Interest:* There are no conflicts to declare.

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