INVESTIGATIONS OF THE MOST ACTIVE COMPOUND AS ANTI-DENTAL CARIES BETWEEN CHEMICAL CONSTITUENTS OF MISWAK

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ABSTRACT

The present study deals with quantum calculations to investigate some chemical descriptors of the main components of miswak extract to evaluate the most potent agents that used as anti dental caries between all the chemical components present in this plant. The chemical descriptors such as HOMO, LUMO, Energy gap, softness, hardness and electrophilicity was used as indicators to evaluate the activity of each component. Using hyperchem-8 package, density functional theory (DFT) was used as quantum method at the basis set L631G* with B3LYP function as the exchange–correlation. It can be concluded that benzyl isothiocyanate is considered as the potent agent that prevent dental careis due to the comparison of several chemical descriptors studied by DFT method.

KEY WORDS: miswak, DFT, anti-dental caries, chemical compositions.

INTRODUCTION

The potent activity of miswak as antioxidant agent come from its ability to scavenge DHHP and ABTS radicals in addition to the synergistic effect when combines with the natural antioxidant enzymes present in the oral such as peroxidase enzyme [1]. Both Salvadora persica and phenolic mouth washes have the same activity as dental plaque reduction and their activity to prevent the inflammation of gingival, while 8 days using of miswak can be reduced the dental plaque 75% [2-3]. Oral hygiene and periodontal diseases of teeth prevention can be attained by using Salvadora persica according to its anti-cariogenic activity and availability, simpilicity and its low cost [4-6]. synergistic effect of combination of miswak and Kalonji can be used to increase the antioxidant activity[7]. Chemical and mechanical effects of miswak are considered the important reason of the potent therapeutic properties of this plant. The mechanical properties include antiplaque and anticalculus in addition to cleansing, while the chemical properties include, antimicrobial, antioxidant, anti-inflammatory and hydrating activities [4, 8-10]

Miswak is considered as good mediated to synthesis eco-frindly silver nanoparticles (AgNPs) due to the reducing agent property, which overcome the uses of toxic chemical reducing agents used for synthesis (AgNPs) [11]. miswak can be used for oral hygiene management of orthodontic patient and to prevent tooth decay [12-13]

Benzyl-isothiocyanate is considered the main constituents' active chemical compounds of miswak, it inhibits the growth and acid streptmutans production and prevent acid increase

Chemical compositions of miswak:

Different chemical components were observed in miswak by different researchers and the main one is benzyl-isothiocyanate which is more than 70% between all the components, then the rest of the materials come in different proportions such as benzaldehyde, benzyl nitrile, and others [14-22] as shown in table-1.)

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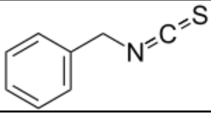
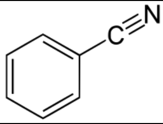
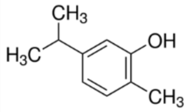
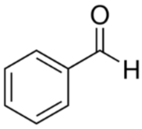
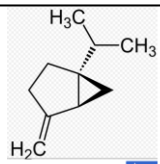
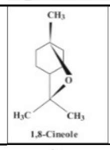
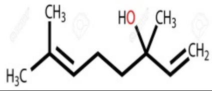
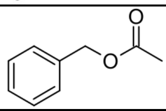
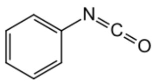
Table (1):- chemical compositions of miswak

No.	Compounds	Chemical Structure
1	Benzylisothiocyanate	
2	Benzylnitrile	
3	Carvacrol	
4	Benzaldehyde	
5	Sabinene	
6	1,8-cineole	
7	Linalool	
8	Benzyl ester	
9	Benzylisocyanate	

Computational details

The hyperchem 8 professional was used as program package. Density functional theory (DFT) was used as molecular modeling at 631G** basis sets (large size basis sets), The use of six Gaussian primitives (631G) to each core orbital improves significantly the description of the core region. B3LYP as hybrid functional was used. All the calculations are carried out at restricted Hartree-Fock levels (RHF).

Chemical descriptors were calculated according to different equations as follow [23-30]:

The hardness (η) was computed by using the following Eq:

$\eta = (E_{LUMO} - E_{HOMO})/2$ ……(1)

Electrophilicity (ω) was calculated from the Eq.:

$\omega = (E_{HOMO} + E_{LUMO}/2)^2/2\eta$. …..(2)

Softness (S) was calculated by:

$S = 1/2\eta$ ……(3)

RESULTS AND DISCUSSION

Chemical descriptors

There is a good relationship between HOMO-LUMO energy gap of the molecule and its chemical reactivity, the low value of Egap, the high active molecule (25-27), Hard molecule means that the molecule is more resistance to polarization, so it is less active when the value is high [28], While soft molecule reveals the ability of electron transfer to another molecule and the high value of softness means more active [29]. Electrophilicity measures the energy lowering of a molecule due to maximal electron flow between the donor and acceptor, so high value of electrophilicity reflects more active molecule [29-30]

From table-2, it can be concluded from the above consideration that benzyl isothiocynate (which is the higher percentage in miswak and reachs more than 70%) is considered the potent active between all the other chemical constituents of miswak, and this result is matched with several experimental studies [14, 31]. The potency of benzyl isothiocynate come from the activity of both nitrogen and sulfur atoms which are considered as active functional groups in addition to benzyl group [32].

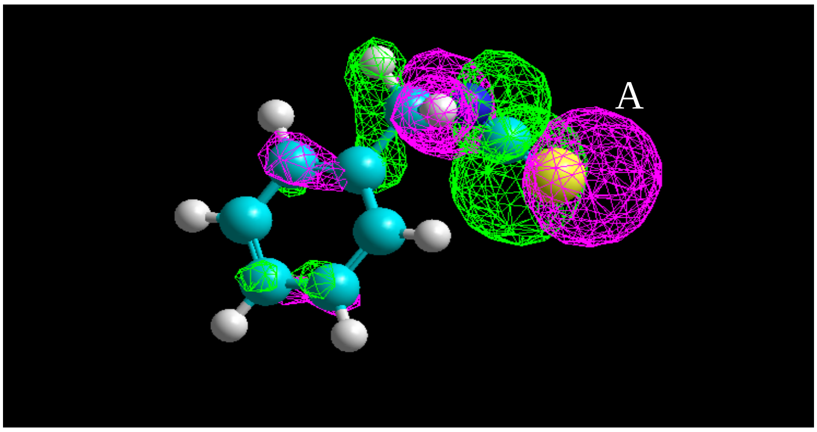
Benzyl isothiocynate can inhibit the growth of *Streptococcus mutans* (which is the main source of dental caries, and has fungi static action toward *Candida albicans* [33]

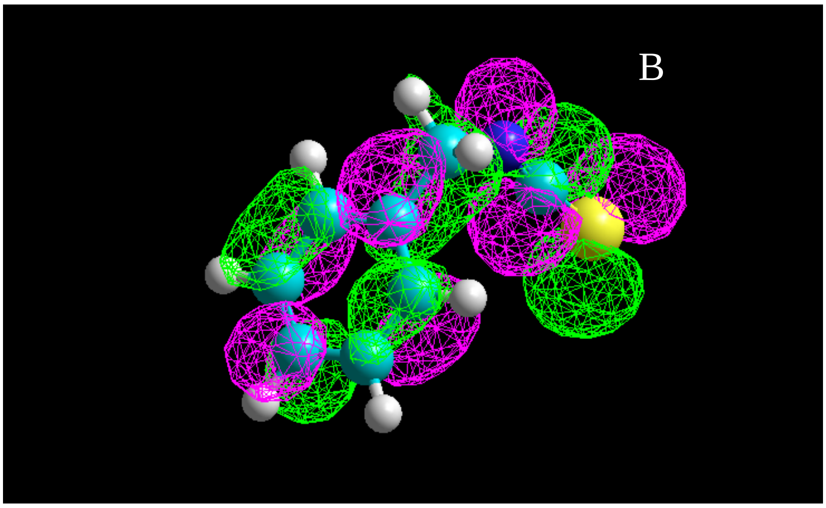
Table(2):- the chemical descriptors of different compsitions present in miswak using DFT/ 631G**/ B3LYP

NO.	Compounds	HOMO eV	LUMO eV	Egap eV	Hardness eV	Electrophilicity eV	Softness eV
1	Benzylisothiocyanate	-6.506	-0.666	5.84	2.920	2.201	0.342
2	Benzylnitrile	-6.955	-0.395	6.56	3.280	2.058	0.304
3	Carvacrol	-6.753	1.619	8.372	4.186	0.787	0.238
4	Benzaldehyde	-6.494	-0.407	6.087	3.043	1.955	0.328
5	Sabinene	-5.956	0.709	6.665	3.332	1.032	0.300
6	1,8-cineole	-6.205	1.865	8.07	4.035	0.583	0.247
7	Linalool	-5.847	0.373	6.22	3.110	1.204	0.321
8	Benzylester	-6.624	-0.138	6.486	3.243	1.762	0.308
9	Benzylisocyanate	-6.768	-0.215	6.553	3.276	1.860	0.305

HOMO LUMO shapes

The shapes of homo lumo are shown Fig-1 , it can be seen that homo is localized over the molecule except benzene ring while lumo is localized above all the molecule which indicates the electrons transferred to benzene ring due to pi-pi* transition.

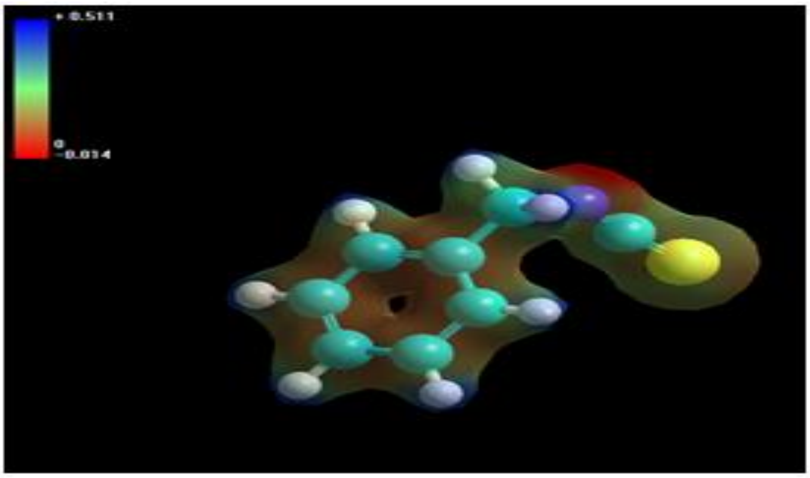




Fig(1): -Benzyl isothiocyanat orbitals, HOMO (A), LUMO (B)

Molecular electrostatic potential (MEP)

To investigate the nucleophilic and electrophilic attacks of the molecule and to describe the electron distribution on the reactive sites of system, (MEP) was used for this purpose which depends on the variation of colors visualized in MEP that is ranged from red color (as negative charge that reflects the electrophilic capacity value) to blue color as positive charge. As can be seen in fig-2 , the electrophilic potency is localized on nitrogen atom which represent the more active site toward electrostatic attacks with the receptor (34):



Fig(2):- Molecular electrostatic potential (MEP) of benzyl isothiocyanat

CONCLUSION

When there is a matching pattern in the results, and when the molecules are sequenced in being the most softness and electrphilicity and the least hardness, this means a high accuracy in determining the most effective substance, so benzylisothiocyanate can inhibit *Streptococcus mutans* which is the main reason of dental caries

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