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QUANTIUM THEORICAL ANALYSIS OF MORINGA AND NITROGENOUS BASES OF DNA AND RNA

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ABSTRACT

Moringa (Mo) is used as traditional medicine in different parts of the world. This work aims to treat by theoretical means and using quantum chemistry to show if the main components of this plant work as it has been tried to study. The main capacity of the Mo is that it works as an anti-inflammatory, being effective for the treatment of diabetes, arthritis and other diseases in muscles and bones. In the last two decades, many reports have appeared in leading scientific journals that describe their nutritional and medicinal properties. The aim of this study is to separate the scientific evidence from the anecdotes found in different articles, whether they are scientific or not. There is not enough information to support the qualities described by the majority of the population. The parts of the leaves were tested for pharmacological activities, namely, antioxidants, antimicrobials, antidiabetics, hypertension, anticancer, anti-inflammatory and others.

KEYWORDS: Moringa, DNA, RNA, Quantum chemistry.

INTRODUCTION

The Moringa oleifera, known as Mo, is a tree native to northern India. It grows on almost any type of soil, even in conditions of high seasonal aridity.

Each 100 g of pod with seeds contains 86.9 g of water; 2.5 g of proteins; 0.1 g of fat, 8.5 g of carbohydrates, fiber 4.8 g, 2.0 g of ash; 30 mg of calcium, 110 mg of phosphorus, 5.3 mg of iron, 184 IU of vitamin A, 0.2 mg of niacin, 120 mg of ascorbic acid, 310 µg of copper and

1.8 µg of iodine. The core of the seed contains 38.4 g of crude protein and 34.7% of fatty oil. The seed oil contains 9.3% palmitic acid, 7.4% stearic acid, 8.6% behenic acid and 65.7% oleic acid. Myristic and lignoceric acids have also been reported among the fatty acids.[1]

The leaves contain per 100 g: 75 g of water, 6.7 g of protein, 1.7 g of fat, 14.3 g of carbohydrates, 0.9 g of fiber, 2.3 g of ash, 440 mg of calcium, 70 mg of phosphorus, 7 mg of iron, 110 µg of copper, 5.1 µg of iodine, 11,300 IU of vitamin A, 120 µg of vitamin B, 0.8 mg of nicotinic acid, 220 mg of ascorbic acid and 7, 4 mg of tocopherol.[2] Estrogenic substances are found, including the antitumor compound β-sitosterol and a pectin esterase. Previous research shows a possible help to solve problems of food insecurity and prevent multiple pathologies associated with deficiencies of vitamins, proteins, minerals, carbohydrates and lipids.[3]

Pods and seeds are useful for water purification. They contain a cationic electrolyte that has proven effective in the treatment of water (elimination of turbidity), replacing aluminum sulfate or other flocculants.[4] The advantage of using these seeds is twofold: it replaces imported products with an easily accessible local one and, unlike aluminum sulphate, is completely biodegradable.[5]

In the ITSON (Technological Institute of Sonora) there have been innovative studies on Mo, among which we can mention:

• Chitosan hydrogels as a support for the peptide extracted from the Mo oleifera seed in water treatment.

• Application of the beads of chitosan and Mo oleifera peptide in water treatment.

• Development and validation of an HPLC analytical method for the quantification of sterols in Mo oleifera.

• Characterization of Mo oleifera seed proteins by electrophoresis and HPLC.

Essential amino acids

Isoleucine, leucine, lysine, methionine, phenylalanine, threonine, tryptophan, valine.

Non-essential amino acids

Alanine, arginine, aspartic acid, cysteine, glutamine, glycine, histidine, proline, serine, tyrosine.

Content of vitamins and minerals of the Mo:[6-9]

Table 1: Values per 100 grams of edible portion.		
COMPOUND	**FRESH LEAVES**	**DRY LEAVES**
Carotene (Vit. A)	6.78 mg	18.9 mg
Thiamin (B1)	0.06 mg	2.64 mg
Riboflavin (B2)	0.05 mg	20.5 mg
Niacin (B3)	0.8 mg	8.2 mg
Vitamin C	220 mg	17.3 mg
Calcium	440 mg	2, 003 mg
Calories	92 cal	205 cal
Carbohydrates	12.5 g	38.2 g
Copper	0.07 mg	0.57 mg
Fat	1.70 g	2.3 g
Fiber	0.90 g	19.2 g
Iron	0.85 mg	28.2 mg
Magnesium	42 mg	368 mg
Match	70 mg	2914 mg
Potassium	259 mg	1324 mg
Protein	6.70 g	27.1 g
Zinc	0.16 mg	3.29 mg

Tabla 2: Nutritional Value per 100 gr. Energy 65 kcal. 270 KJ.	
Carbohydrates	8.28 g
Fat (trimiristina)	1.40 g
Water	78.66 g
Proteins	9.40 g
Dietary Fiber	2 g

The ETC theory

The BG is defined as the energy difference between the valence band and the conduction band. In the BG there are no electronic states available; this means that when an electric field is applied the electrons cannot increase their energy.

In quantum theory, it is known as HOMO and LUMO, and in the old theory they are known as E- and E +. The LUMO is defined as the range of electronic energy that allows acceleration in electrons by the presence of electrical currents and is also called conduction band; HOMO is defined as the highest energy interval that is occupied by electrons in absolute zero value and is called valence band. The HOMO is the most electron-filled orbital, while the LUMO is the orbital that lacks electrons. The HOMO equaled to zero (HOMO 0) is the last layer full of orbitals meaning that it is in the last valence orbital. The LUMO equaled to zero (LUMO 0) is the last layer that lacks electrons.

EP is defined as the total potential energy of the molecule. It is an electrostatic field vector that is defined as the potential that the electron needs to jump the Bohr radius (0.53 Armstrong) by its calculated natural electromotive force (EMF). The negative E value (E-) is the electrostatic potential with negative poles, while the positive E value (E +) is the proton-electron potential. The EP, in other words, means that having 1 EP is having 1 volt for Armstrong. The EP is obtained by the absolute difference of E- and E +.

The ETC is defined as the dimensionless parameter that describes an electrochemical reaction, which is interpreted as the number of times the potential energy needs to jump to the BG. It is calculated by dividing the BG and the EP entirely. That is, if it has a BG of 10 and an ETC of 40, it means that you need 40 times the EP value in EV so that the BG of 10 jumps from the HOMO to LUMO.

MATERIALS AND METHODS

SE-PM3 is a program for molecular modeling used by scientists to analyze the quantum composition of molecules for HOMO-LUMO, BG, EP and other properties. These data are used to form the table where are the ETC´s of the interaction between the Lev and the Nitrogenous Bases (NB). El Software Hyperchem Professional performs Molecular modeling and analysis of the Lev and the NB. (Hyperchem, hypercube, Multi in for Windows, series 12-800-1501800080.) (Multi in South 1236-301 Tlacoquemecatl Insurgentes Col. del Valle, Benito Juárez, DF, Mexico C.P. 03200).

Table 3: Parameters used for quantum computing molecular orbitals-HUMO and LUMO.

Parameter	Value	Parameter	Value
Total charge	0	Polarizability	Not
Spin Multiplicity	1	Geometry Optimization algorithm	Polak-Ribiere (Conjugate Gradient)
Spin Pairing	RHF	Termination condition RMS gradient of	0.1 Kcal/Amol
State Lowest Convergent Limit	0.01	Termination condition or	1000 maximum cycles
Interaction Limit	50	Termination condition or	In vacuo
Accelerate Convergence	Yes	Screen refresh period	1 cycle

Table 4: Parameters used for visualize the map of the electrostatic potential of the molecules.

Parameter	Value	Parameter	Value
Molecular Property	Property Electrostatic Potential	Contour Grid increment	0.05
Representation	3D Mapped Isosurface	Mapped Function Options	Default
Isosurface Grid: Grid Mesh Size	Coarse	Transparency level	A criteria
Isosurface Grid: Grid Layout	Default	Isosurface Rendering: Total charge density contour value	0.015
Contour Grid: Starting Value	Default	Rendering Wire Mesh	

RESULT AND DISCUSSIONS

The analysis of table 5 shows the changes in the comparison that were made in the bases in the compounds of natural Mo presenting the ETC less than Ca. The tables and graphs of the relevant compounds with lower ETC are observed.

Table 6 shows the crossing of ETC bands with the compounds found in the Mo and the DNA and RNA bases. Only those lower values of ETC are taken, which are the ones that present a more probable reaction.

Table 6: Mo crossbands Vs NB.

Number	Reducing agent	Oxidizing agent	Interacción	ETC
1	adenine	BETA CAROTENE	adenine -- BETA CAROTENE	31.0352161
2	THIAMINE	thymine	THIAMINE -- thymine	30.6919699
3	THIAMINE	uracile 1	THIAMINE --uracile 1	30.2471565
4	PYRIDOXINE (B6)	uracile 2	PYRIDOXINE (B6)--uracile 2	30.1314467
5	THIAMINE	uracile 2	THIAMINE--uracile 2	29.1745121
6	adenine	ALFA CAROTENO	adenine --ALFA CAROTENE	27.9468908
7	cytosine	RIBOFLAVIN	cytosine--RIBOFLAVIN	27.827282
8	RETINOL	thymine	RETINOL--thymine	27.3660135
9	guanine	RIBOFLAVIN	guanine--RIBOFLAVIN	27.1797172
10	RIBOFLAVIN	thymine	RIBOFLAVINE--thymine	27.0575779
11	RETINOL	uracile 1	RETINOL--uracile 1	26.9832699
12	RIBOFLAVIN	uracile 1	RIBOFLAVIN--uracile 1	26.7003802
13	adenine	RIBOFLAVIN	adenine --RIBOFLAVIN	26.33639
14	adenine	FRUCTOSE	adenine --FRUCTOSE	26.2080863
15	cytosine	THIAMINE	citosine--THIAMINE	26.0957829
16	RETINOL	uracile 2	RETINOL--uracile 2	26.088408
17	RIBOFLAVIN	uracile 2	RIBOFLAVIN--uracile 2	25.8652975
18	guanine	THIAMINE	guanine--THIAMINE	25.4106346
19	PYRIDOXAMINE (B6)	uracile 2	PYRIDOXAMINE (B6)--uracile 2	25.3890277
20	cytosine	RETINOL	citosine--RETINOL	25.2446676
21	adenine	THIAMINE	adenine --THIAMINA	24.6798665
22	adenine	PYRIDOXAL (B6)	adenine --PYRIDOXAL (B6)	24.6091156
23	guanine	RETINOL	guanine--RETINOL	24.5540183
24	adenine	ASCORBIC Ac. (VC)	adenine -- ASCORBIC Ac. (VC)	24.1721753
25	adenine	RETINOL	adenine --RETINOL	23.8831864
26	adenine	PYRIDOXAL PHOSPHATE (B6)	adenine -- PYRIDOXAL PHOSPHATE (B6)	22.6897123
27	adenine	P	adenine --P	22.3882707
28	adenine	Fe	adenine --Fe	17.5186946
29	adenine	Ca	adenine --Ca	9.90885103
30	uracile 2	Zn	uracile 2--Zn	2.17991653
31	NIACIN (B3)	thymine	NIACIN (B3)--thymine	1.30572979
32	uracile 2	Mg	uracile 2--Mg	0.46057143

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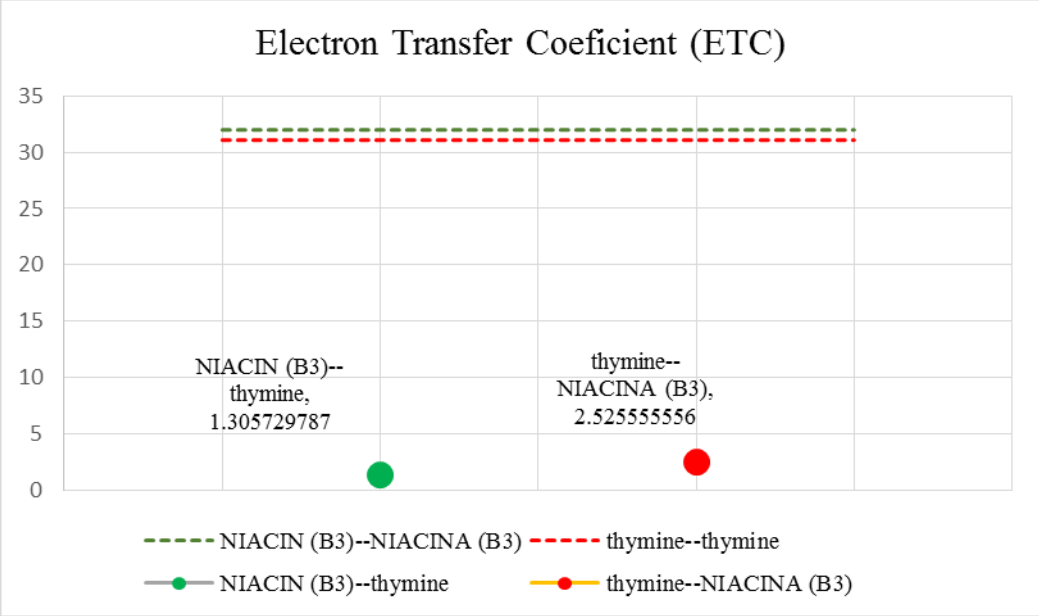

Fig. 1: Quantum Well Niacin Vs Thymine.

The percentage of energy needed for a reaction to occur between the compounds of lower ETC of niacin and thymine is represented in figure 1. The quantum well with the lower and upper limits is very small and the plotted points show that the more below the limits is found the reaction will be more likely.

Table 7: ETCs and probability of the most significant interactions occurring.

Type of interaction	Reducing agent	Oxidizing agent	Interaction	ETC	Limits
Pure Substance	RIBOFLAVIN	RIBOFLAVIN	RIBOFLAVIN--RIBOFLAVIN	29.2132353	**Higher**
	uracile 2	uracile 2	uracile 2--uracile 2	29.0900246	**Lower**
Crossband	RIBOFLAVIN	uracile 2	RIBOFLAVINE--uracile 2	25.8652975	
	uracile 2	RIBOFLAVIN	uracile 2--RIBOFLAVIN	32.8356726	

Table 7 shows the amount of energy transfer coefficient necessary for a reaction to occur between the compounds. The uracil present in the RNA has the lowest ETC as long as it

works as an oxidizing agent, which is better for Riboflavin to enter as an antioxidant agent that helps the body to be metabolized.

CONCLUSIONS

1. The compounds present in Mo are mostly vitamins that can be metabolized by the body.
2. The minimum values of ETC present are the highest levels of reaction between the compounds of Mo and the NB.
3. All compounds show a high solubility with NB.
4. No foreign compound is present inside the plant, which could mean that not all the properties that they present are true.
5. The compounds have a reaction in DNA and RNA as shown in the general table
6. They can bind both adenine and uracil 1 and 2.
7. It can be presented as vitamin complexes.

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