https://doi.org/10.46344/JBINO.2023.v12i01.17

STUDY OF THE CHEMICAL-QUANTUM INTERACTIONS OF ERYTHROIDINE AND AMINO ACIDS IN THE HUMAN BODY

[1,2] **Manuel González-Pérez,** [1]**Adriana Reyes-Castro,** [1]**Laura Rodríguez-Peláez,** [1]**Jesús Antonio Salazar-Magallón,** [1]**Pedro Antonio Rodríguez-Salazar,** [1]**Juventino Reza-Salgado.**

[1]Universidad Tecnológica de Tecamachalco (UTTCAM). Ingeniería en Agricultura Sustentable y Protegida.

[2]Tecnológico Nacional de México, Campus Tepeaca (TecNM Campus Tepeaca). Ingeniería en Industrias Alimentarias.

E-mail: investigacionvinc@uttecam.edu.mx, m.gonzalez.perez@personal.uttecam.edu.mx

ABSTRACT

β-erythroidine have been isolated and structurally characterized from the methanolic extract of the stem bark of E. poeppigiana. These alkaloids have found anticancer properties at specific receptors. This investigative work aimed to find the antioxidant chemical-quantum interactions of erythroidine (ETI) vs. amino acids (AAs) in the human body. The Hamiltonian combinatorial theory was used to perform all valence electron jumps between each substance, atom by the atom of each molecule. We use Hyper Chem's parametrized semi-empirical model number 3 (SE-PM3) to draw the corresponding molecules. We then selected SE-PM3. He optimized the geometry with the Polak Ribiere method. The oxidation of ETI by molecular oxygen occurs with greater probability and chemical affinity, while oxidation with water occurs with medium probability. The quantum chemical interactions of ETI-AAs demonstrate the antioxidant properties of ETI.

Keywords: Quantum Chemistry, Hyperchem, Erythroidine, Amino acids, Electron transfer coefficients.

1. INTRODUCTION

1.1 ETI and cancer.

In recent yeaDjiogue et al. (2014) isolated and structurally characterized four erythroidine alkaloids, namely a-erythroidine, β-erythroidine and their oxo-derivatives 8-oxo-a-erythroidine, and 8-oxo-β-erythroidine of the methanolic extract of the stem bark of E. poeppigiana. They found that a-erythroidine and β-erythroidine showed ERa binding affinity values of 0.015 ± 0.010% and 0.005 ± 0.010%, respectively, whereas only β-erythroidine bound ERβ (0.006 ± 0.010%). The results were confirmed in MVLN cells, a bioluminescent variant of MCF-7 breast cancer cells. Both a-erythroidine and β-erythroidine induced enhanced expression of specific ERa-dependent genes, clover factor-1, and serum/glucocorticoid-regulated kinase 3 in MCF-7 cells, confirming estrogenicity.

Hikita et al. (2017) showed that erypoegin K, isolated from the stem cortex of Erythrina poeppigiana, has a potent apoptosis-inducing effect in cancer cell lines, such as HL-60. They concluded that its cytotoxic effect was much stronger than known glyoxalase I inhibitor Sp-bromobenzylglutathione cyclopentyl diester. They say that treatment of HL-60 cells with erypoegin K significantly induced caspase-3 activity, whereas pretreatment of cells with caspase-3 inhibitor suppressed erypoegin K-induced cell death. On the other hand, they conclude that nuclear condensation and DNA fragmentation of the apoptotic genome were observed in HL-60 cells treated with Erypoegin K.rs, some alkaloids such as erythroidine, and a-erythroidine.

1.2 Erythroidine and nicotine.

Nurvita et al. (2022) investigated the possible effects of E.subumbrans (Hassk.) Merr. Extract on nicotine withdrawal syndrome and β2 nAChR expression in the ventral tegmental area (VTA) of rats. They found that a 100 mg/kg BW dose can decrease some somatic signs in nicotine-smoking patients.

1.3 Erythroidine and receptors.

Sallam (2022), Williams and Robinson (1984), De Mora (2020), and Yu (202) report that the nicotinic cholinergic antagonist, dihydro-beta-erythroidine, binds to two sites on rat cortical membranes with dissociation constants. of 4 and 22 nM and respective apparent Bmax values of 52 and 164 fmol/mg protein. Binding to the highest affinity site, defined using 2 nM [3H] dihydro-beta-erythroidine, was saturable, reversible, and susceptible to protein denaturation. 8. These findings indicate that dihydro-beta-erythroidine binds to a nicotinic recognition site in the rat brain that is neuromuscular, rather than ganglionic, in nature and that such binding is similar in several respects to that observed with nicotinic agonists.

1.4 Erythroidine toxicity.

Mateos and Vázquez (2000) evaluated the toxicity of alkaloid fractions obtained from the E, American seed in vitro in some crustaceans, such as Daphnia magna and Artemia salina, in the bacterium Bacillus cereus, and the nematode Panagrellus redivivus. They found that the toxicity of the hexanoic and methanolic fractions of free alkaloids in Daphnia magna, Artemia salina, Bacillus cereus, and Panagrellus redivivus was different from that induced by the alkaloid fraction released from E. Americana seeds. The presence of a and β-erythroidines was detected in the fractions. The released alkaloid fraction turned out to be the most toxic, especially with identifying erysopine, erysodine, and erysovine alkaloids. The crustacean Daphnia magna and the nematode Panagrellus redivivus presented a higher sensitivity to the extracts tested than the remaining organisms.

2. MATERIAL AND METHODS

2.1 Hamiltonian technique.

The hamiltonian combinatorial theory performed all the valence electron jumps

between each substance, atom by an atom of each molecule.

2.2 Quantum methodology:
The molecular simulator Hyper Chem (HC) was purchased. (Hyper Chem. Hypercube, MultiON for Windows. Serial #12-800-1501800080. MultiON. Insurgentes Sur 1236 - 301 Tlacoquemecatl Col. del Valle, Delegación Benito Juárez, D. F., México CP. 03200).

We use the Hyper Chem parameterized semi-empirical model number 3 (SE-PM3) to draw the corresponding molecules. We then selected SE-PM3. He optimized the geometry with the Polak Ribiere method. He calculated the variables of HOMO-LUMO, BG, EP, and other properties. The results are displayed in column-delimited tables for each concept used in the calculations.
The specific parameters selected for each simulation were the following: SET UP. Semi-empirical method: PM3. Semiempirical Options: Load and Spin. Total Load 0. Multiplicity Turn 1. SCF Control. Convergent limit 0.01. Interaction Limit 1000. Speed Up Converge Yes. Lowest matchmaking spin. Superimposition of weighting factors Sigma-

3. RESULTS AND DISCUSSION

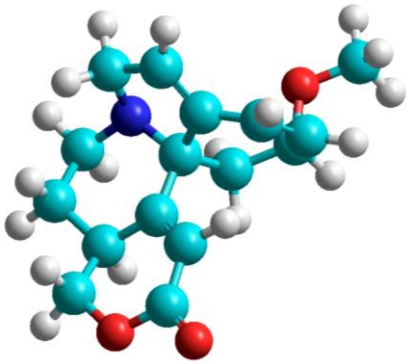
3.1 Characterization.
Figure 1 shows us four characteristics of the erythroidine molecule. All quantum calculations are based on these four features—the characterization of the erythroidine molecule with hyperchem.

Sigma 1, Pi-Pi1. Polarizabilities were not calculated.

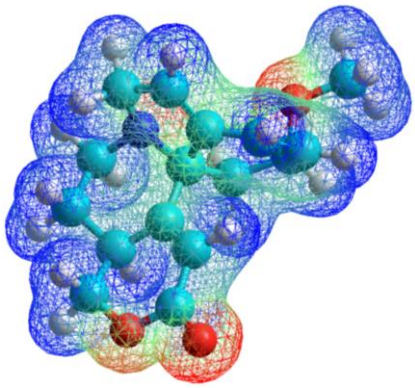
CALCULATION 1. Geometry optimization. Polak Ribiere algorithm (conjugate gradient). Options Termination conditions. RMS gradient of 0.1 kcal/mol or 1000 cycles maximum. Empty, yes. Screen update period one cycle.

CALCULUS 2. Orbitals. Plot orbital options Isosurface representation. Orbital contour value 0.05. Wire mesh isosurface grid. Grid meshes size Coarse. Default grid layout. Default beam contour. Transparency level Default.

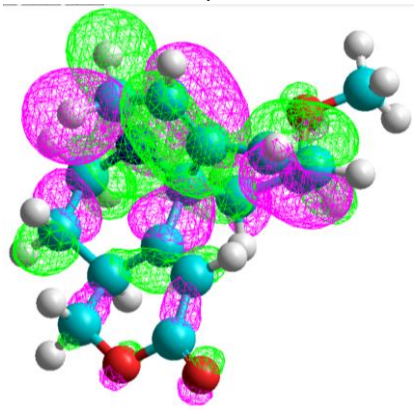
CALCULATE 3. Molecular drawings and calculations. Plot molecular options. Molecular Properties. Properties. Electrostatic potential Yes. Representations. Isosurface mapped in 3D. Grid meshes size Coarse. Default grid layout. Irregular Curve Default. Rereading of Isosurfaces. Total Charge Density Contour Value (TCDCV) 0.015. Wire mesh. Transparency level Default. Assigned options Default functions. González et al (2017,2017,2022)



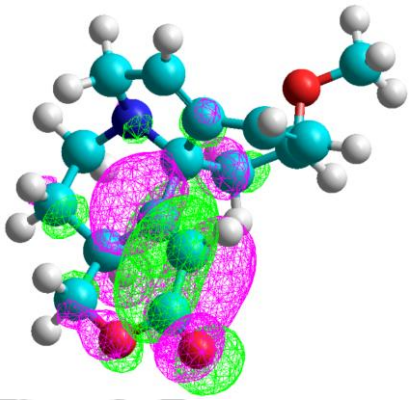
A) a- erythroidine E = -4083.2889 kcal/mol



B) δ- = -0.132 eV/a°, δ+ = 0.128 eV/a°



C) HOMO = -9.162407 eV



D) LUMO = -0.3405294 eV

Figure 1. A) H white, C cyan, N blue, O red. B) Electrostatic map. δ- red, δ+ blue, δ (neutral) green. C) Orbital most occupied by valence electrons. D) Least busy orbital.

One of the significant results is shown in table 1. In this table, the interaction between molecular oxygen and erythroidin is exhibited. It is observed that the interaction between Erythroidine vs. O_2 has an ETC = 30.298 a° (Bohr radii). This interaction is at the bottom of the table (quantum well), meaning it is the most probable and the most similar of all.

Table 1. ETCs of the interaction of O_2 and erythroidin.

DATA	Name	Reducing agent	Oxidizing agent	HOMO	LUMO	Bg	δ-	δ+	EP	ETC
48	Oxygen	O_2	O_2	-10.733	-0.982	9.751	-0.038	0.138	0.176	55.403
588	Erythroidine	ETID	ETID	-9.162	-0.341	8.822	-0.132	0.128	0.260	33.930
Option 1	**Oxygen vs. Erythroidine**	**O_2**	**ETID**	**-10.733**	**-0.341**	**10.392**	**-0.038**	**0.128**	**0.166**	**62.605**
Option 2	**Erythroidine vs. Oxygen**	**ETID**	**O_2**	**-9.162**	**-0.982**	**8.180**	**-0.132**	**0.138**	**0.270**	**30.298**

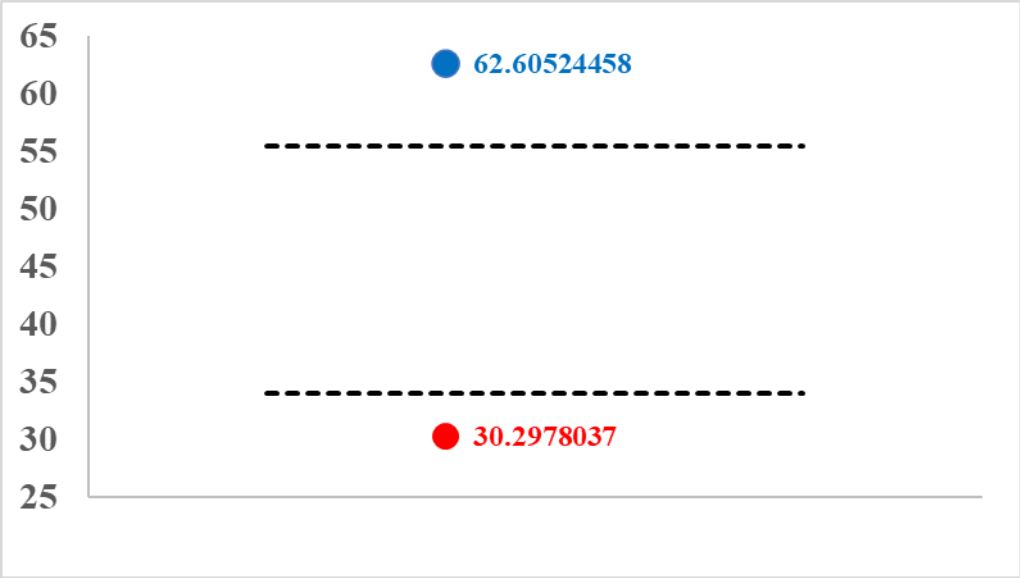


Figure 2 best exemplifies this phenomenon.

In this figure 2, the dotted lines represent the ETCs of the pure substances to have interacted. These lines are the ETCs limits. Below the lower dotted line is the area of most excellent affinity and probability. In the middle of the dotted lines is the zone of medium probability. Above the upper dotted line is the area with the slightest probability that the phenomenon will occur. The Erythroidine vs. O2 interaction is represented by the red dot and is located at the bottom of the quantum well. Therefore, the oxidation of erythroidine by molecular oxygen occurs with greater probability and chemical affinity.

Table 2 is like Table 1, but the interaction is with water. It is observed that both the oxidative interaction and the reductive interaction remain in the middle zone.

Table 3. ETCs of the interaction of O_2 and erythroidin.

DATA	Name	Reducing agent	Oxidizing agent	HOMO	LUMO	Bg	δ–	δ+	EP	ETC
47	Water	H_2O	H_2O	-12.316	4.059	16.375	-0.127	0.171	0.298	54.950
588	Erythroidine	ETID	ETID	-9.162	-0.341	8.822	-0.132	0.128	0.260	33.930
Option 1	**Water vs. Erythroidine**	**H_2O**	**ETID**	**-12.316**	**-0.341**	**11.975**	**-0.127**	**0.128**	**0.255**	**46.963**
Option 2	**Erythroidine vs. Water**	**ETID**	**H_2O**	**-9.162**	**4.059**	**13.221**	**-0.132**	**0.171**	**0.303**	**43.635**

Figure 3 shows the interactions of erythroidine and water. It is observed that oxidation (red dot) predominates over antioxidation (blue dot), according to Table 2. In this case, water predominates as the oxidizing agent.

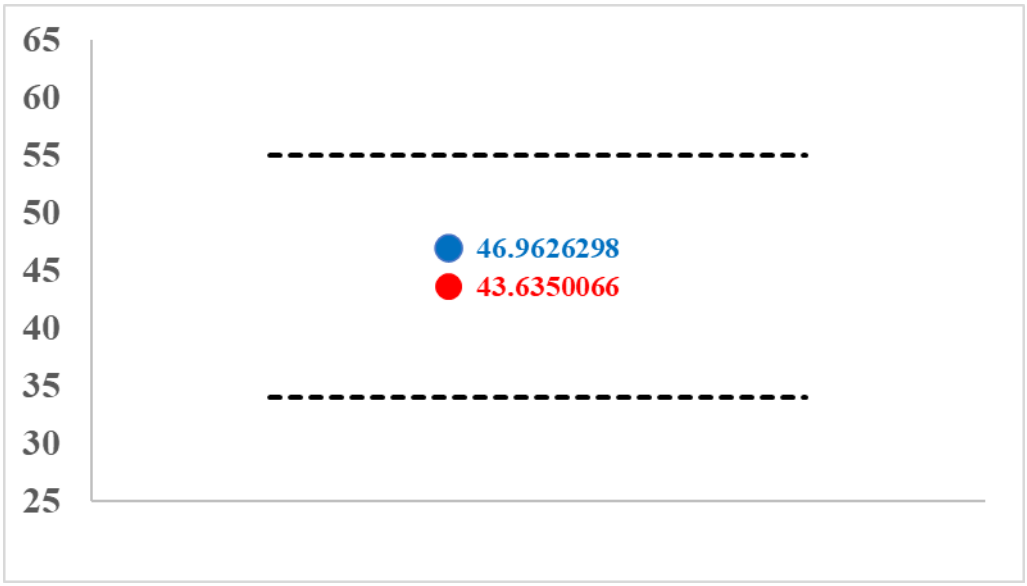


Figure 3. Erythroidine vs. Water. Water oxidizes erythroidine with medium chemical affinity and probability.

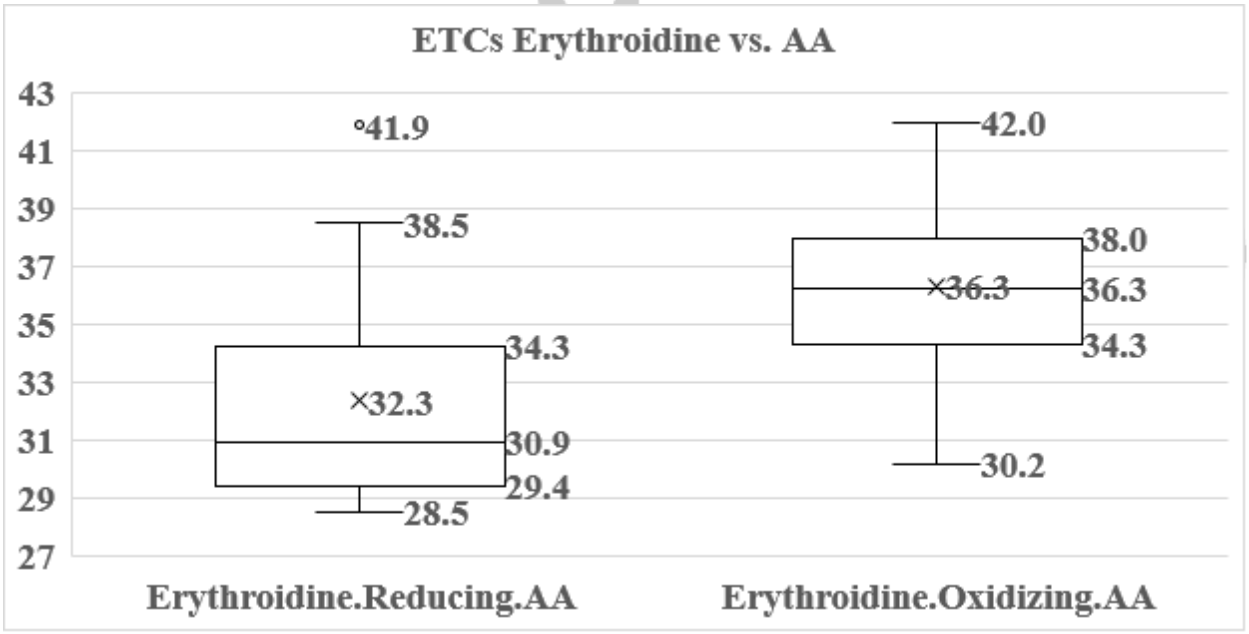


Figure 4. Interactions of redox erythroidin vs. AA. It is observed that reduction reactions (antioxidants) predominate due to their lower location in the quantum well.

In figure 4, we can see two whisker diagrams. The first diagram shows us the antioxidant interactions of erythroidine and amino acids. The second diagram represents the oxidative interactions of erythroidine and amino acids. It is evident to see that the first diagram is located lower than the second diagram. This situation leads us to think that the antioxidant interactions of erythroidine vs. amino acids are more related, probable, and robust.

5. CONCLUSIONS

5.1 Hypothesis.

The erythroidine compound, derived from bunting, has antioxidant properties for amino acids in the human body.

5.2 Thesis.
The antioxidant properties of erythroidine are demonstrated with the quantum-chemical interactions with the whisker diagram in figure 3.

5.3 Corollary and arguments.
All these quantum calculations are available (emails from the corresponding author).
Oxygen was found to be a powerful oxidizing agent for erythroidine, while water is a medium oxidizing agent.

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