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CHEMICAL-QUANTUM STUDY OF POLYVINYLPYRROLIDONE COLLAGEN VS AMINO ACIDS OF EPITHELIAL TISSUE IN DIABETIC PATIENTS

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ABSTRACT

Quantum chemistry is a branch of science based on quantum mechanics and the quantum theory of magnetic fields. It describes the behavior of metal in interaction with the energy that composes it (electrons, protons, and neutrons). These interactions are achieved with the help of specific mathematical calculations for each compound. Electrostatic Coefficient Theory (ETC) is defined as the dimensionless parameter that describes an electrochemical reaction, which is interpreted as the number of times that potential energy must jump to the band gap (BG). It is calculated by completely dividing the BG and the electrostatic potential (EP). The interaction that requires less energy is found with AA Ser present in epithelial tissue. ACCORDING TO THE ETC THEORY, the AA that continues to be under lower electrical potential is Gln, Pro, and Lys. The AA Gln, Pro, and Lys with low ETC indicate a favorable interaction reaction with the PVPCOLAG compound. In conclusion, the low probability of reaction between BN and PVPCOLAG is beneficial. It means that the possibility of altering the DNA or RNA chains is low when the PVPCOLAG comes into contact with epithelial tissue cells. The quantum well between AA and PVPCOLAG is smaller than the quantum well of BN. There is a possibility that the reaction time between AA and PVPCOLAG is shorter when they interact together.

KEYWORD : Chemical-quantum, Polyvinylpyrrolidone, Collagen, Epithelial tissue, Diabetic patients

INTRODUCTION

Quantum chemistry is a branch of science based on quantum mechanics and the quantum theory of magnetic fields. Describes the behavior of metal in interaction with the energy that composes it (electrons, protons, and neutrons). Quantum chemistry is achieved with the help of specific mathematical calculations for each compound with which it is desired to interact. [1]

Collagen is a set of fibrous proteins found in the matrix of bones, teeth, cartilage, tendons, nails, skin, and blood vessels. The fundamental unit of collagen is the tropocollagen formed by three polypeptide chains of similar size, each one of them is a left-handed helix, and they are intertwined with each other; The type of chain that forms the tropocollagen determines the type of collagen. Collagen comprises 33% glycine, 12% proline, 20% hydroxyproline, and 10% hydroxylysine, present in only some proteins. [2] The primary function of collagen is to maintain the structure of animal tissues and improve the tissues' strength, resistance, and flexibility. [3]

Polyvinylpyrrolidone (PVP) is an inert polymer that is practically non-metabolizable and is mainly excreted via the urine (95%) in less than 24 hours. It is very soluble in water, with a solubility of 100 mg/ml. In the dry state, it can absorb up to 40% of its weight in water. PVP couples with iodine, serving as a carrier to take advantage of the disinfecting action. [4]

Within pharmacodynamics, the data generated from in vitro studies suggest that PVPCOLAG acts at the level of fibroblasts and macrophages, modulating collagen metabolism. In such a way, said regulation participates in the reparative processes with a better quality and response time in healing. [5]

PVPCOLAG is a biopharmaceutical that regulates healing processes and modulates the inflammatory response that affects acute, subacute, and chronic conditions. [6] It favors the replacement of connective tissue components. In addition to increasing the tissue regeneration process, it improves the quality of the scar by eliminating the deposited collagen, ruling out the possibility of obtaining a keloid or hypertrophic scar. [7]

PVPCOLAG is a component derived from porcine skin collagen in a citrate solution that stabilizes its pH. It contains an inert polymer (polyvinylpyrrolidone) that enhances its effect. [8]

AAs are substances that the body requires to make specific proteins needed. These can be essential or nonessential, meaning that the body must consume or produce those that the body can produce. Among its functions are those of repairing body tissues. The AA present in epithelial tissue is Glutamine (Gln), Glycine (Gly), Isoleucine (Ile), Leucine (Leu), Lysine (Lys), Proline (Pro), Serine (Ser), and Valine (Val). These interact to keep the cells in good condition. They work with the platelet system and with the tissue factor in case of needing tissue healing. [9]

Diabetes mellitus (DM) is a metabolic disorder characterized by the presence of chronic hyperglycemia that is accompanied, to a greater or lesser extent, by alterations in the metabolism of carbohydrates, proteins, and lipids.

Wounds in diabetic patients are a frequent problem that occurs in the population. The multiple complications such as nerve damage, skin fragility, problems in wound healing, causing poor quality of life in the patient. Functional limitations, pain, discomfort, inflammation, or even patient mortality. [10]

One of the complications in patients with diabetes mellitus (DM) is the diabetic foot. The diabetic foot includes several syndromes. The interaction of loss of protective sensation due to sensory neuropathy, change in pressure points due to motor neuropathy, autonomic dysfunction, and decreased blood flow due to peripheral vascular disease results in minor trauma, induced injury, or ulcers that go unnoticed. [eleven]

The PVPCOLG aims to accelerate the regeneration process of damaged tissue by interacting with the AA that makes up the epithelial tissue. It will reduce the risk of infection due to antimicrobial activity, decrease inflammation and pain in the area.

The research's general objective is to study the reaction generated between PVPCOLAG and AA using quantum chemistry. Quantum studies demonstrate the interaction with BN to analyze the interaction between these compounds. Some scientists are looking at these studies

as a benefit for interaction with AA. In turn, these calculations generate the possible improvement in the response with other drugs available for the pathology of diabetes mellitus I-II.

MATERIALS Y METHODS

ETC (Electrostatic Coefficient Theory) is the dimensionless parameter describing an electrochemical reaction, which is interpreted as the number of times potential energy must jump to the BG. [10] It is calculated by completely dividing the BG and the EP. [12]

LUMO is defined as the range of electrical energy that allows the acceleration of electrons by electrical currents and is also called the conduction band. HOMO is the highest energy interval that electrons occupy at an absolute zero value called the valence band. HOMO is the most electron-filled orbital, while LUMO is the lowest-electron orbital. HOMO equal to zero (HOMO 0) is the entire last shell of orbitals, which means it is in the last valence orbital. LUMO, equal to zero (LUMO 0), is the last shell that lacks electrons. [13]

BG is the energy difference between the valence band and the conduction band. In the BG, there are no electronic statements available; This means that when an electric field is applied, the electrons cannot increase their energy. [14]

EP is defined as the total potential energy of the molecule. An electrostatic field vector is a potential the electron needs to

jump the Bohr radius (0.53 Armstrong) by its calculated natural electromotive force (EMC). The negative E value (E-) is the electrostatic potential with negative poles, while the positive E value (E +) is the electron-proton potential [6]. The EP, in other words, means that having 1 EP has 1 volt for Armstrong. The absolute difference of E gets EP- and E +. [15]

SE-PM3 is a molecular modeling program used by scientists to analyze the quantum

composition of molecules for HOMO-LUMO, BG, EP, and other properties. These data form the table where the ETC of the interaction between Lev and NB is found. Hyperchem professional software performs molecular and analytical models of Lev and NB. (Hyperchem, hypercube, Multi in for Windows, series 12-800-1501800080) (Multi en Sur 1236-301 TlacoquemecatI Insurgentes Col. del Valle, Benito Juárez, DF, México C.P. 03200). [16]

Table 1. 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 2. Parameters used for visualizing 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	

It is essential to know the band crossing of the compounds tested individually and calculate a minuscule amount when the compound acts as a reducing agent or an

oxidizing agent. In this way, the binding reports that the compounds are interacting with each other. This observation will

depend on which compounds interact and the relationship between them. [17]

RESULT AND DISCUSSIONS

The present analyses of the interacting compounds are CPP, DNA-RNA nitrogenous bases, and the AAs in the skin

necessary for the healing process. These are; Glutamine (Gln), Glycine (Gly), Isoleucine (Ile), Leucine (Leu), Lysine (Lys), Proline (Pro), Serine (Ser), and Valine (Val). The AA present in the study is those with which the ETC concentration is lower interacting with PVPCOLAG.

Table 3 presents the calculations of the leading compounds of the study.

Table 3. ETC calculations for AA and CPP compounds

No.	Reducing agent	Oxidizing agent	HOMO	LUMO	BG	E-	E+	EP	ETC
9	Val	Val	-9.913814	0.9311865	10.845001	-0.131	0.109	0.24	45.187502
8	PVPCOLAG	PVPCOLAG	-9.370077	0.8924601	10.262537	-0.123	0.117	0.24	42.760571
7	Leu	Leu	-9.645295	0.9220657	10.567361	-0.126	0.13	0.256	41.278753
6	Gly	Gly	-9.902413	0.9015826	10.803996	-0.137	0.159	0.296	36.499985
5	Ser	Ser	-10.15642	0.5648013	10.721221	-0.108	0.198	0.306	35.036671
4	Ile	Ile	-9.872066	0.971656	10.843722	-0.128	0.188	0.316	34.315576
3	Gln	Gln	-10.0231	0.7548746	10.777975	-0.124	0.192	0.316	34.107515
2	Lys	Lys	-9.520605	0.9427313	10.463336	-0.127	0.195	0.322	32.494833
1	Pro	Pro	-9.446512	0.7919495	10.238462	-0.128	0.191	0.319	32.095491

Compounds that require a lower concentration of ETC are observed in the table, leading to a greater possibility of interaction since the energy load to be used is less than the central compound (PVPCOLAG).

Table 4. ETC interaction between AA and PVPCOLAG

No.	Reducing agent	Oxidizing agent	HOMO	LUMO	BG	E-	E+	EP	ETC
25	Ser	PVPCOLAG	-10.15642	0.8924601	11.0488801	-0.108	0.117	0.108	102.304445
24	Gln	PVPCOLAG	-10.0231	0.8924601	10.9155601	-0.124	0.117	0.241	45.2927805
23	Val	Val	-9.913814	0.9311865	10.8450005	-0.131	0.109	0.24	45.1875021
22	PVPCOLAG	Val	-9.370077	0.9311865	10.3012635	-0.123	0.109	0.232	44.4019978
21	Ile	PVPCOLAG	-9.872066	0.8924601	10.7645261	-0.128	0.117	0.245	43.9368412
20	Val	PVPCOLAG	-9.913814	0.8924601	10.8062741	-0.131	0.117	0.248	43.5736859
19	Leu	PVPCOLAG	-9.645295	0.8924601	10.5377551	-0.126	0.117	0.243	43.3652473
18	PVPCOLAG	PVPCOLAG	-9.370077	0.8924601	10.2625371	-0.123	0.117	0.24	42.7605713
17	Lys	PVPCOLAG	-9.520605	0.8924601	10.4130651	-0.127	0.117	0.244	42.6764963
16	Gly	PVPCOLAG	-9.902413	0.8924601	10.7948731	-0.137	0.117	0.254	42.4995004
15	Pro	PVPCOLAG	-9.446512	0.8924601	10.3389721	-0.128	0.117	0.245	42.1998861

14	Leu	Leu	-9.645295	0.9220657	10.5673607	-0.126	0.13	0.256	41.2787527
13	PVPCOLAG	Leu	-9.370077	0.9220657	10.2921427	-0.123	0.13	0.253	40.6804059
12	Gly	Gly	-9.902413	0.9015826	10.8039956	-0.137	0.159	0.296	36.4999851
11	PVPCOLAG	Gly	-9.370077	0.9015826	10.2716596	-0.123	0.159	0.282	36.4243248
10	Ser	Ser	-10.15642	0.5648013	10.7212213	-0.108	0.198	0.306	35.0366709
9	Ile	Ile	-9.872066	0.971656	10.843722	-0.128	0.188	0.316	34.3155759
8	Gln	Gln	-10.0231	0.7548746	10.7779746	-0.124	0.192	0.316	34.1075146
7	PVPCOLAG	Ile	-9.370077	0.971656	10.341733	-0.123	0.188	0.311	33.2531608
6	Lys	Lys	-9.520605	0.9427313	10.4633363	-0.127	0.195	0.322	32.4948332
5	PVPCOLAG	Lys	-9.370077	0.9427313	10.3128083	-0.123	0.195	0.318	32.4302148
4	PVPCOLAG	Pro	-9.370077	0.7919495	10.1620265	-0.123	0.191	0.314	32.3631417
3	PVPCOLAG	Gln	-9.370077	0.7548746	10.1249516	-0.123	0.192	0.315	32.1427035
2	Pro	Pro	-9.446512	0.7919495	10.2384615	-0.128	0.191	0.319	32.0954906
1	PVPCOLAG	Ser	-9.370077	0.5648013	9.9348783	-0.123	0.198	0.321	30.9497766

The purpose of the interactions in table 4 is to recognize those compounds that require a lower concentration of energy to achieve the interaction between them.

The PVPCOLAG compound, when working as an antioxidant, manages to combine with the AA compounds.

Table 5. ETC calculation interaction between BN and PVPCOLAG

N	Reducing agent	Oxidizing agent	HOMO	LUMO	BG	E-	E+	EP	ETC
22	Water	Water	-12.316	4.059	16.375	-0.127	0.171	0.298	54.9496644
21	PVPCOLAG	Water	-12.316	0.8924601	13.2084601	-0.127	0.117	0.244	54.1330332
20	Water	PVPCOLAG	-9.370077	4.059	13.429077	-0.123	0.171	0.294	45.6771327
19	thymine	PVPCOLAG	-9.71045	0.8924601	10.6029101	-0.124	0.117	0.241	43.9954776
18	Uracil 1	PVPCOLAG	-9.71046	0.8924601	10.6029201	-0.127	0.117	0.244	43.4545906
17	PVPCOLAG	PVPCOLAG	-9.370077	0.8924601	10.2625371	-0.123	0.117	0.24	42.7605713
16	Uracil 2	PVPCOLAG	-9.881824	0.8924601	10.7742841	-0.136	0.117	0.253	42.5861032
15	Cytokine	PVPCOLAG	-9.142321	0.8924601	10.0347811	-0.16	0.117	0.277	36.2266466
14	Guanine	PVPCOLAG	-8.537118	0.8924601	9.4295781	-0.145	0.117	0.262	35.9907561
13	Adenine	PVPCOLAG	-8.555917	0.8924601	9.4483771	-0.155	0.117	0.272	34.7366805
12	PVPCOLAG	Cytokine	-9.370077	-0.3436248	9.0264522	-0.123	0.154	0.277	32.58647
11	PVPCOLAG	Adenine	-9.370077	-0.2342397	9.1358373	-0.123	0.165	0.288	31.7216573
10	Thymine	Thymine	-9.71045	-0.5107842	9.1996658	-0.124	0.172	0.296	31.079952
9	PVPCOLAG	Guanine	-9.370077	-0.2061208	9.1639562	-0.123	0.176	0.299	30.6486829
8	Uracil 1	Uracil 1	-9.71046	-0.5107848	9.1996752	-0.127	0.176	0.303	30.3619644
7	PVPCOLAG	thymine	-9.370077	-0.5107842	8.8592928	-0.123	0.172	0.295	30.031501
6	PVPCOLAG	Uracil 1	-9.370077	-0.5107848	8.8592922	-0.123	0.176	0.299	29.6297398
5	Uracil 2	Uracil 2	-9.881824	-0.427566	9.454258	-0.136	0.189	0.325	29.0900246
4	PVPCOLAG	Uracil 2	-9.370077	-0.427566	8.942511	-0.123	0.189	0.312	28.6618942
3	Cytokine	Cytokine	-9.142321	-0.3436248	8.7986962	-0.16	0.154	0.314	28.0213255
2	Adenine	Adenine	-8.555917	-0.2342397	8.3216773	-0.155	0.165	0.32	26.0052416
1	Guanine	Guanine	-8.537118	-0.2061208	8.3309972	-0.145	0.176	0.321	25.9532623

The interaction of ETC vs. BN and PVPCOLAG present in table 5 demonstrates the energy required by the compounds to interact with each other. What is feasible for this interaction is that

no change occurs between the compounds. If there were a possible interaction between the compounds in Table 5, it would have the possibility of presenting some mutation in the BN.

Table 6. Compound combination (Cross Band) of Ser and PVPCOLAG

Substance type	Reducing agent	Oxidizing agent	Interaction	ETC	Limits
Highest interaction	Ser	PVPCOLAG	Ser--PVPCOLAG	102.3044454	Higher limit of interactions
Pure substance 1	PVPCOLAG	PVPCOLAG	PVPCOLAG--PVPCOLAG	42.76057125	Higher
Pure substance 2	Ser	Ser	Ser--Ser	35.03667092	Lower
Lower interaction	PVPCOLAG	Ser	PVPCOLAG--Ser	30.94977664	Lower limit of interactions

Table 6 shows the combination of ETCs among the compounds that represent the most significant possibility of chemical interaction between them. The theory mentions that the lower the amount of ETC, the lower the range of jump to the

counting well the compounds to be analyzed will present, representing better energy to achieve chemical-quantum stability.

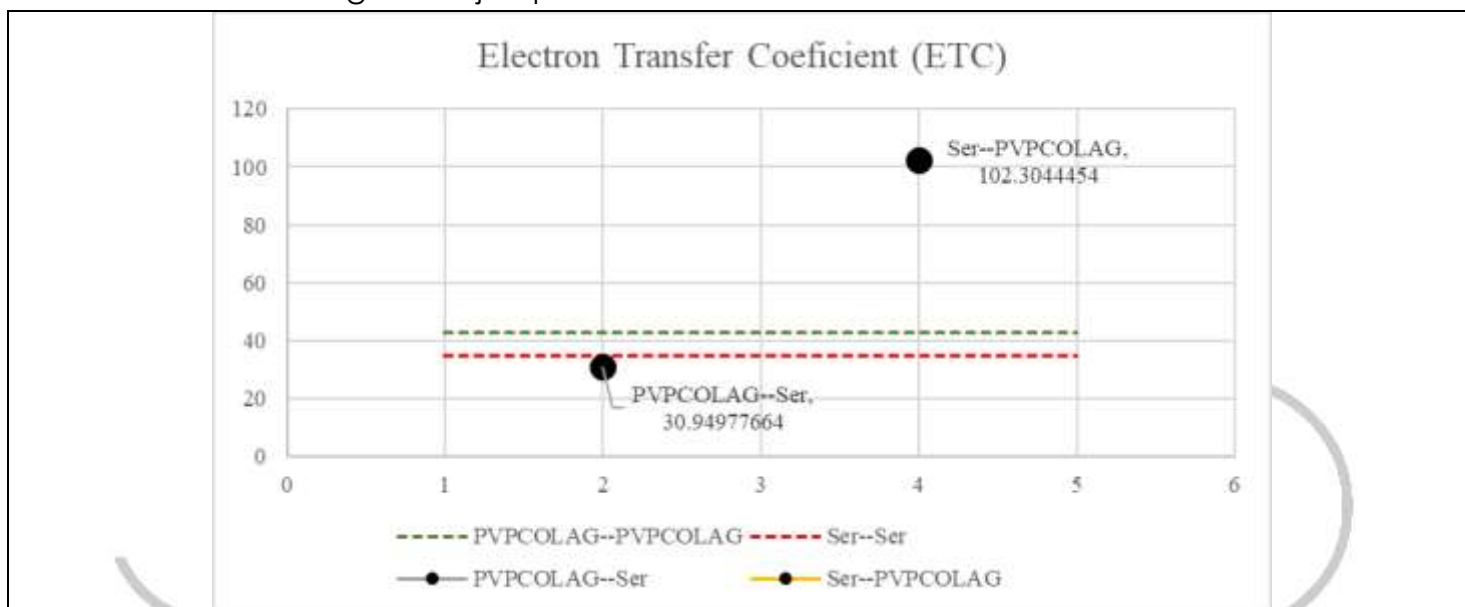


Figure 1. Quantum well of interaction between the compounds PVPCOLAG and Ser

The percentage of energy required for a reaction between the compounds with lower ETC is presented in figure 1. These are Ser-PVPCOLAG. The quantum well at its

lower and upper limits is tiny, and the plotted points show the interaction or combination between them. This lowest point indicates the stability of the bond.

Table 7. Combination of compounds (Cross Band) of PVPCOLAG and Gln.

Substance type	Reducing agent	Oxidizing agent	Interaction	ETC	Limits
Highest interaction	PVPCOLAG	PVPCOLAG	PVPCOLAG--PVPCOLAG	42.76057125	Higher limit of interactions
Pure substance 1	Gln	Gln	Gln--Gln	34.10751456	Higher
Pure substance 2	PVPCOLAG	Gln	PVPCOLAG--Gln	32.14270349	Lower
Lower interaction	Gln	PVPCOLAG	Gln--PVPCOLAG	45.2927805	Lower limit of interactions

Table 7 shows the energy concentration interaction (ETC) combination for the compounds PVPCOLAG and Gln. The interaction occurs in less quantity while PVPCOLAG works as a reducing chemical compound, an antioxidant.

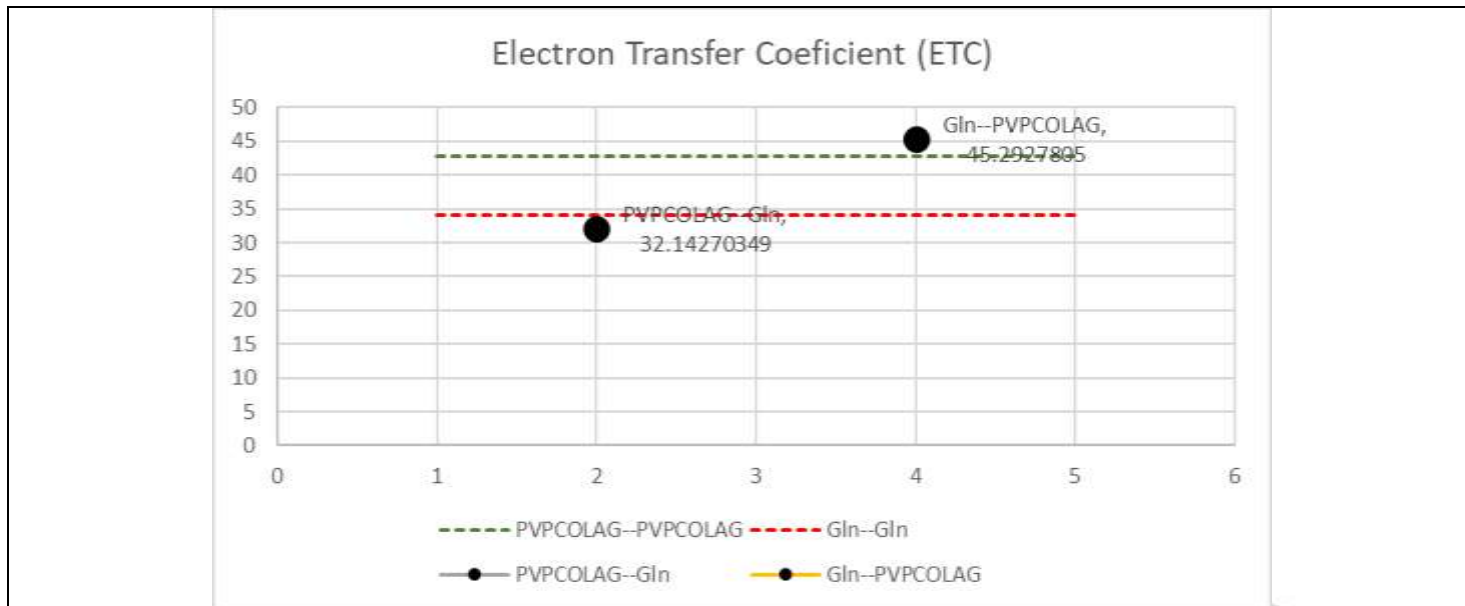


Figure 2. Quantum well of interaction between the compounds PVPCOLAG and Gln.

Figure 2 of the AA Gln shows the probable interaction zone at the lower concentration when the PVPCOLAG molecules come into contact.

Table 8 and Figure 3 show the probable zone of interaction between the compounds to be studied. AA shows affinity due to the lower concentration of energy it requires to interact.

Table 8. Combination of compounds (Cross Band) of PVPCOLAG and Lys

Substance type	Reducing agent	Oxidizing agent	Interaction	ETC	Limits
Highest interaction	PVPCOLAG	PVPCOLAG	PVPCOLAG--PVPCOLAG	42.76057125	Higher limit of interactions
Pure substance 1	Lys	Lys	Lys--Lys	32.49483323	Higher
Pure substance 2	PVPCOLAG	Lys	PVPCOLAG--Lys	32.43021478	Lower
Lower interaction	Lys	PVPCOLAG	Lys--PVPCOLAG	42.67649631	Lower limit of interactions

The energy measured in the compounds mentioned above derives from the charge that electrons release during the excitation process when they meet other chemical

substances that we want to study. The case of compound Lys with PVPCOLAG is shown in table 8 and figure 3.

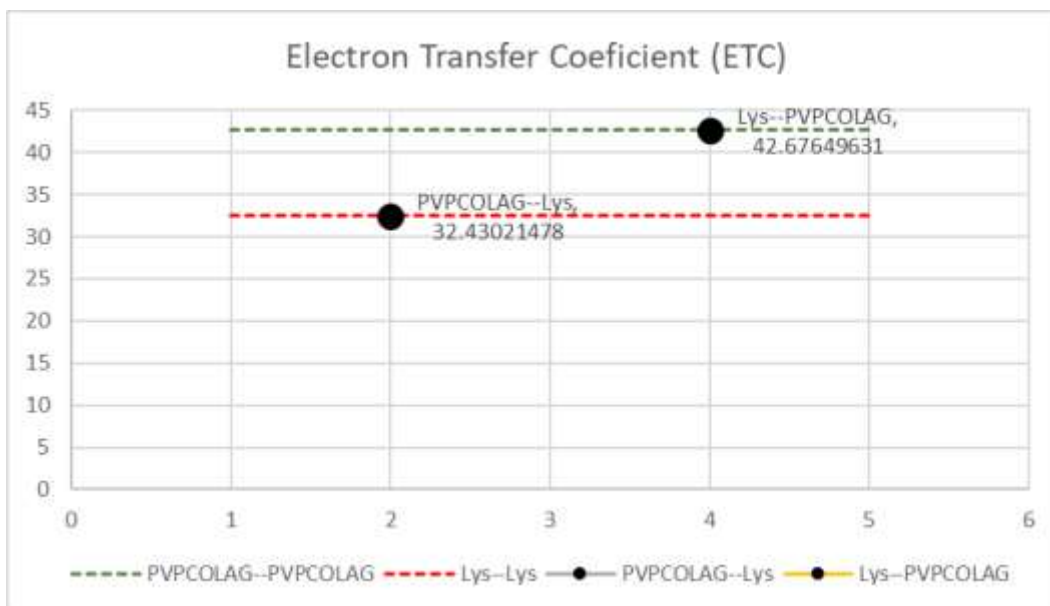


Figure 3. Quantum well of interaction between the compounds PVPCOLAG and Lys

Table 9. Combination of compounds (Cross Band) of PVPCOLAG and Pro.

Substance type	Reducing agent	Oxidizing agent	Interaction	ETC	Limits
Highest interaction	PVPCOLAG	PVPCOLAG	PVPCOLAG--PVPCOLAG	42.76057125	Higher limit of interactions
Pure substance 1	Pro	Pro	Pro--Pro	32.0954906	Higher
Pure substance 2	PVPCOLAG	Pro	PVPCOLAG--Pro	32.36314172	Lower
Lower interaction	Pro	PVPCOLAG	Pro--PVPCOLAG	42.19988612	Lower limit of interactions

The compounds in Table 9 and Figure 4 describe the high probability of interaction between them. When presenting this interaction, the short distance between the plotted points is observed in the graph. This

observation shows that the quantum well to "jump" from the electron to join the compound will have lower electrical potential.

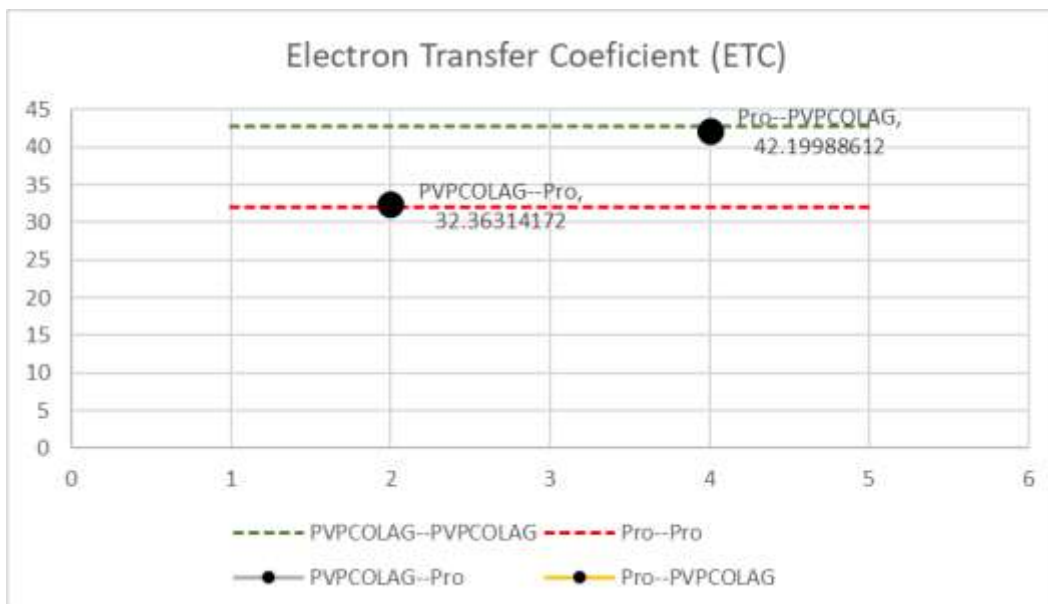


Figure 4. Quantum well of interaction between the compounds PVPCOLAG and Pro

CONCLUSION

1. The interaction that requires less energy is found with AA Ser present in epithelial tissue.
2. ACCORDING TO THE ETC THEORY, the AA that continues to be under lower electrical potential is Gln, Pro, and Lys.
3. The AA Gln, Pro, and Lys with low ETC indicate a favorable interaction reaction with the PVPCOLAG compound.
4. Theoretically and quantumly, AAs with a lower concentration of ETC work as an oxidant when they come into contact with PVPCOLAG.
5. PVPCOLAG has a favorable reaction as an antioxidant or reducer when interacting with the AA of the epithelial tissue.
6. The reaction with BN and PVPCOLAG presents a high amount of ETC, which implies that the energy required to

combine both compounds is more significant than that of AA.

7. Higher concentrations between compounds generate little probability of reaction between them.
8. The low probability of reaction between BN and PVPCOLAG is beneficial. It means that the possibility of altering the DNA or RNA chains is low when the PVPCOLAG comes into contact with epithelial tissue cells.
9. The quantum well between AA and PVPCOLAG is smaller than the quantum well of BN.
10. There is a possibility that the reaction time between AA and PVPCOLAG is shorter when they interact together.

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