

QUANTUM QUANTIC ANALYSIS OF COCAINE INTERACTIONS AND NITROGEN BASES USING THE QUANTUM MODEL SE-PM3

Rodrigo Aramburo-Dartiguez¹, Marisol Villegas-Ruiz¹ and Manuel González-Pérez^{2*}

¹Universidad Popular Autónoma del Estado de Puebla (UPAEP) México. Decanato de ingenierías. Escuela de química. Ingeniería Química Industrial

²Universidad Popular Autónoma del Estado de Puebla (UPAEP) México. Decanato de biología. Escuela de Química.

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***Corresponding Author**

Dr. Manuel González-Pérez

Universidad Popular
Autónoma del Estado de
Puebla (UPAEP) México.
Decanato de biología.
Escuela de Química.

ABSTRACT

Deoxyribonucleic (DNA) acid and ribonucleic acid (ARN) form the basis of our genome. They determine the main essence of each. In this work, we calculate the chemical-quantum interactions of cocaine and contrast them with cross-band interactions with the nitrogenous bases of RNA and DNA. We use hyperchem simulator. The semi-empirical parametric method 3 (SE-PM3). Specifically, to the Polak Ribiere algorithm for the geometrization of the system. The HOMO, LUMO, Bandgap (BG) variables were calculated with the Orbitals algorithm. The calculations for pure substances were made first. Calculations were made in crossed bands of each nitrogenous base vs. cocaine. It was found that cocaine interacts more efficiently with tautomer 2 of uracil due to its lower ETC. In this interaction, cocaine works as an

antioxidant and with a very high probability. Cocaine works as an oxidant of C and G, with a medium probability. The difference between the attack on all the bases is small; therefore, it is concluded that at any given moment, cocaine can attack any of the bases in an oxidative or reducing way.

KEYWORDS: Quantum Chemistry, Cocaine, Nitrogenous Bases, DNA-RNA, SE-PM3.

INTRODUCTION

DNA and RNA form the basis of our genome. They determine the main essence of each.^[1,2]

DNA is found in the nucleus of cells and is composed of the nitrogenous bases: Adenine,

Guanine, Cytosine, and Thymine. RNA allows information encoding DNA. It is formed by a simple chain including uracil instead of thymine.^[3]

Cocaine is a stimulant that directly affects brain functions.^[4, 5] It is produced with the leaves of the coca plant (*Erythroxylum coca*), native to South America. The area of the brain most stimulated by cocaine is the ventral tegmental area (VTA). To generate rewarding stimuli, the nerve fibers that leave the ventral area extend to the nucleus accumbens.^[6] The nerve fibers generate an increase in dopamine levels, increasing neuronal activity in the nucleus accumbens.^[7] In the same way, cocaine prevents the elimination of dopamine, serotonin, and noradrenaline by the synapses of neurons.^[8] Resulting in the accumulation of dopamine in neurons.^[9] Fact that generates euphoria for the consumption of the stimulant. The consumption of cocaine is eliminated in the urine at 3-4 days of consumption, blood in the first two days and hair in a time greater than 90 days.^[10] Cocaine has central effects in the brain 30 seconds after its contact. It is metabolized by enzymatic hydrolysis.

Dopamine is a neurotransmitter of the nervous system, which is more massive amounts generates an increase in heart rate and pressure, loss of sleep, and overactive systems. The dopaminergic neurotransmission system is involved in the processes of cognition, behavior, and emotions of the individual. For this reason, the excessive consumption of cocaine can develop relevant dysfunctions in the individual, generating epigenetic mutations and psychiatric disorders.^[11] The addiction predisposes to other psychiatric conditions such as the abuse of other substances, depression, anxiety, among others.^[12]

In this work, we calculate the chemical-quantum interactions of cocaine and contrast them with cross-band interactions with the nitrogenous bases of RNA and DNA.

MATERIALS AND METHODS

We use hyperchem simulator. The semi-empirical parametric method 3 (SE-PM3). Specifically to the Polak Ribiere algorithm for the geometrization of the system. The HOMO, LUMO, Bandgap (BG) variables were calculated with the Orbitals algorithm. The variables electrostatic negative potential (E-), positive (E +) and potential molecular difference (EP) were calculated with the Plot Molecular Graph algorithm. Finally, the electron transfers coefficient (ETC) is calculated by dividing the bandgap by the electrostatic potential) $ETC = BG / EP$. We group the data into tables, and we plot the quantum wells.^[13-17]

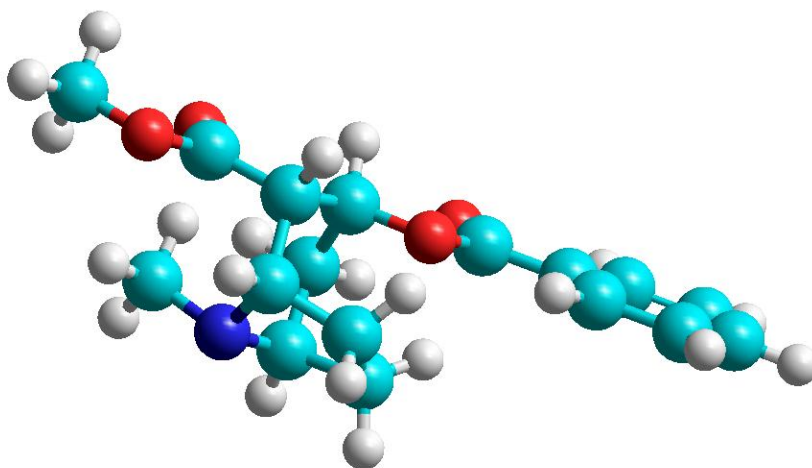


Figure 1. Cocaine molecule in 3D.

The results of the cocaine calculations fig. 1 with the results of the nitrogenous bases and exciting things were observed.

RESULTS AND DISCUSSIONS

Table 1 shows the parameters of the quantum characterization of cocaine. It can be noticed that the ETC = 34.201 is the highest of all the pure nitrogenous bases. These ETCs of the nitrogenous bases are shown in Table 2.

Table 1: Result of the calculations of the quantum parameters characteristic of cocaine.

HOMO	LUMO	BG	E-	E+	EP	ETC
-9.176	-0.523	8.6529	-0.122	0.131	0.253	34.201

Observation 1. Cocaine can attack any nitrogenous base in its pure state. The reason is that it has a higher ETC than all of them. The higher the value of a more unstable ETC is the substance and has higher energy. The ETC works as the impedance in electronics.

In table 2 we can see the interactions of the nitrogenous bases vs. cocaine Note that the most potent interaction is cocaine-U2. By this reason, it has the smallest ETC of all and means a lower impedance and higher conductance for the valence electrons. The interactions of cocaine with C and G respectively follow this rule.

Table 2: Interactions of nitrogenous bases with Cocaine (cross-band).

No.	Reducing agent	Oxidizing agent	HOMO	LUMO	BG	E-	E+	EP	ETC
1	Cocaine	U1	-9.176	-0.511	8.665	-0.122	0.171	0.293	29.572
2	Cocaine	T	-9.176	-0.475	8.701	-0.122	0.169	0.291	29.899
3	A	Cocaine	-8.654	-0.523	8.131	-0.14	0.131	0.271	30.004

4**	Cocaine	U2	-9.176	-0.415	8.761	-0.122	0.202	0.324	27.039
5*	C	Cocaine	-9.142	-0.523	8.619	-0.174	0.131	0.305	28.260
6*	G	Cocaine	-8.537	-0.523	8.0141	-0.15	0.131	0.281	28.520

****Stronger interaction because it is the smallest ETC value of all substances. RNA.**

*** Second and third interaction due to their smaller ETCs, but larger than the previous one**. DNA and, RNA.**

Observation 2. We can observe that cocaine attacks U2 very quickly. It is a sure target. Because U2 is unique to RNA then, cocaine affects RNA as a first target and as a second target to DNA (Table 2).

Table 3: Behavior of nitrogenous bases with cocaine.

Amino Acid	Predominant Action	Probability	Reducing Agent	Oxidizing Agent	ETC
U1	Antioxidant	High	Cocaine	U1	29.57
T	Antioxidant	High	Cocaine	Timina	29.9
A	Oxidant	Medium	A	Cocaine	30
U2 fig.2	Antioxidant	Medium	Cocaine	Adenina	27.04
C fig. 3	Oxidant	Medium	C	Cocaine	28.26
G fig. 4	Oxidant	Medium	G	Cocaine	28.5

Table 3 shows a summary of the probability of occurrence of interactions and their electronic impedance (ETCs).

The difference between the highest ETC and the lowest ETC is small, a little less than three units. This means that any of them can happen at any given time. However, figures 2, 3 and 4 show the quantum wells of the most significant interactions. This means that any of them can happen at any given time. However, figures 2, 3 and 4 show the quantum wells of the most significant interactions. The blue line represents the bottom of the quantum well of the pure interaction of cocaine, while the red line represents the interaction of the clear base in question.

The high probability is located below the red line, the average probability, between the two lines and the high probability, is located above the blue line (figs. 2, 3 and 4).

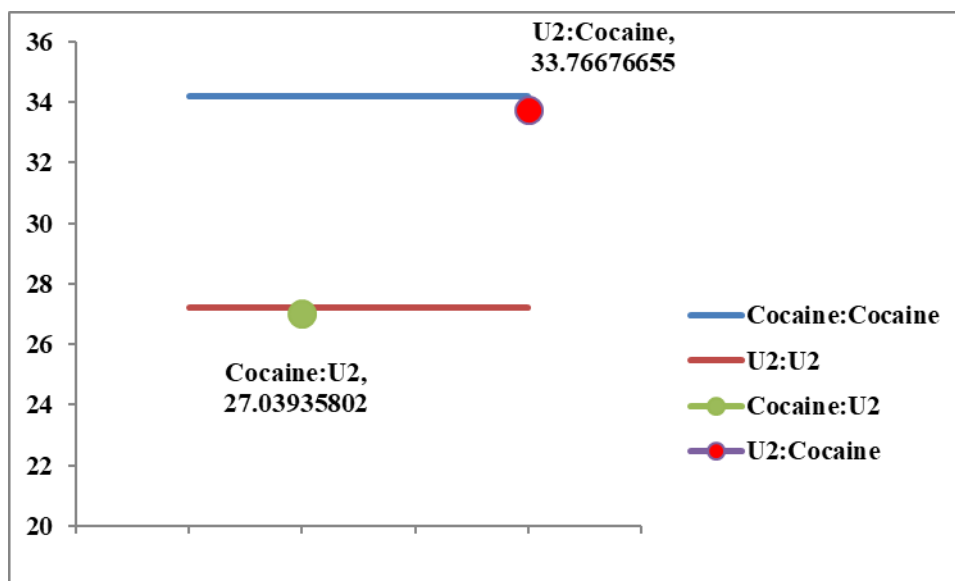


Figure 2. Quantum well of the interaction Cocaine - U2. Although cocaine is reduced, it can produce mutation in the RNA.

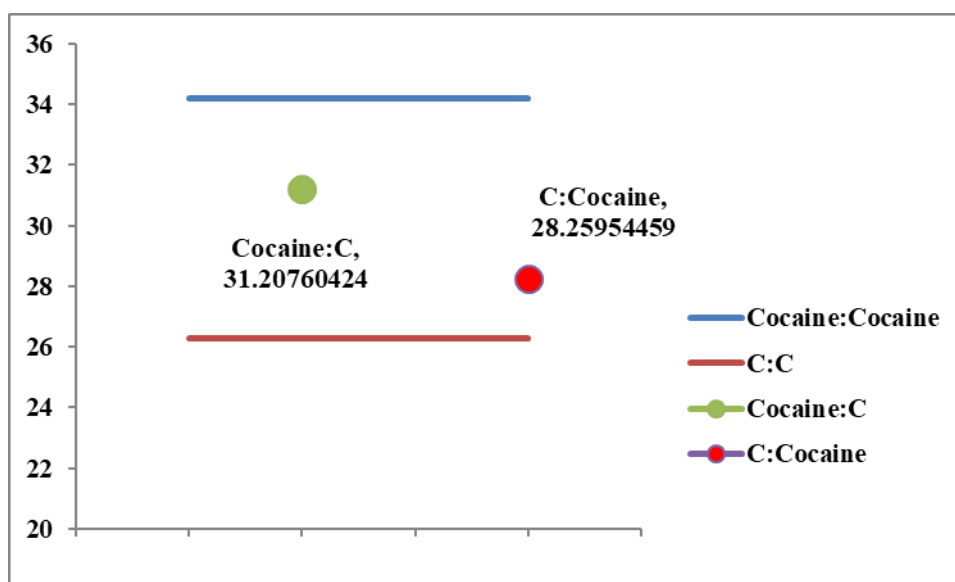


Figure 3. Quantum well of the interaction C - Cocaine. Cocaine oxidizes first to C with medium probability.

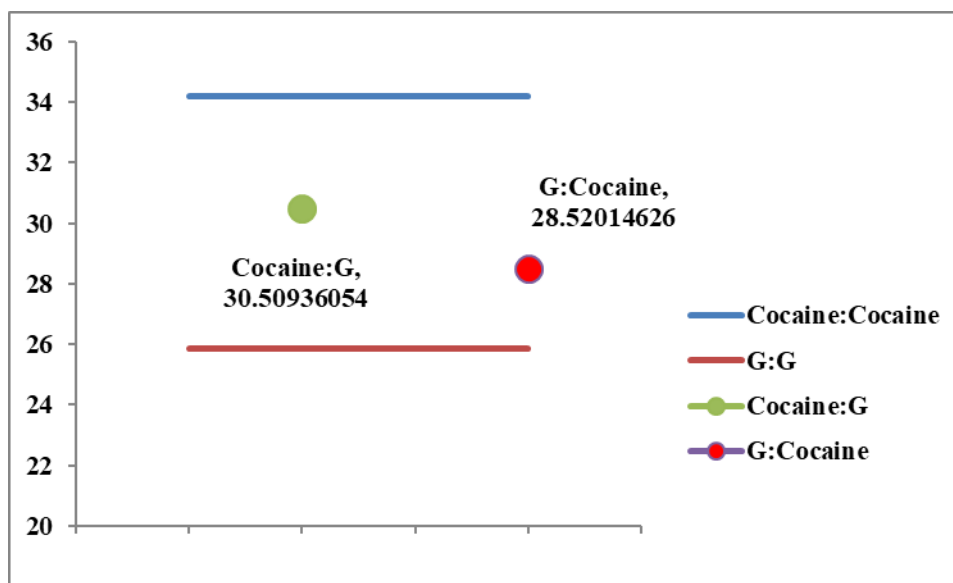


Figure 4. Quantum well of the interaction G - Cocaine. Cocaine oxidizes second to C with medium probability.

CONCLUSIONS

We characterize the quantum parameters of nicotine vs. the nitrogenous bases.

1. The calculations for pure substances were made first.
2. Calculations were made in crossed bands of each nitrogenous base vs. cocaine.
3. It was found that cocaine interacts more easily with tautomer 2 of uracil due to its lower ETC.
4. In this interaction cocaine works as an antioxidant and with a very high probability.
5. Cocaine works as an oxidant of C and G, with a medium probability.

It can be said that cocaine attacks RNA first and then DNA, although the latter attacks it with a medium probability and higher impedance than when it attacks RNA. The difference between the attack on all the bases is small, therefore it is concluded that at any given moment, cocaine can attack any of the bases in an oxidative or reducing way.

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