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ANALYSIS OF THE EFFECT OF STEVIOL VS. NITROGEN BASES OF RNA AND DNA USING QUANTUM METHODS

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ABSTRACT

The main component of the Stevia (STV) is steviol [(5β,8α,9β,10α,13α)-13-Hydroxykaur-16-en-18-oic acid]. In recent years Stevia (STV) has aroused the interest of researchers due to high human consumption as an artificial sweetener. In this work, the general objective was to analyze the chemo-quantum interactions of Steviol and nitrogenous bases. As a result of the lowest interaction of Steviol:U2 is ETC =28,872 because of the high probability that Steviol causes a mutation in RNA. This alteration is similar to that caused by nicotine to RNA as well. Another important observation is that Steviol acts as a reducing agent (antioxidant) in all nitrogenous bases; but, it is not reliable; for its low cross-band ETC with U2. In this way, it can be said that not always that a substance is antioxidant, it is good for health.

KEYWORD: Stevia, Steviol, DNA, RNA, SE-PME, Quantum Chemistry.

INTRODUCTION

In recent years Stevia (STV) has aroused the interest of researchers due to high human consumption as an artificial sweetener. The STV is an herbaceous shrub about 80 cm high; its

leaves accumulate the highest content of glycosides. The level of glycosides in the plant is very variable, with values of 2% and 18% depending on the variety. It used Hyper Chem molecular simulator for Windows Serial # 12-800-1501800080 SE-PM3 for Calculus of ETC.

The properties of STV reported in scientific articles are regulation of glycemic, hypertension, contraception, treatment of skin disorders and in caries prevention[1], stimulates alertness, facilitates digestion, gastrointestinal functions and maintains the feeling of vitality and wellbeing It has been reported that STV has bactericidal effects on *Streptococcus mutans*. This bacterium is responsible for tooth decay.[2] Consumers of STV report are decreasing consumption of tobacco and alcoholic beverages.[3]

Stevia rebaudiana (STVR) PMID: 14561506 is used as a natural sweetener or in dietary supplements for its content of active glycosides present in the leaves (Stevioside and rebaudioside A, B, C, D and E, Dulcoside A and Steviolbioside) with chemical and pharmacological characteristics for human consumption.[3-6]

The complete chemical composition of the STV species is not yet available. In the chemical products found are apigenin, austroinilin, avicularin, β-sitosterol, caffeic acid, campesterol, caryophyllene, centaureidin, chlorogenic acid, chlorophyll, kaempferol, luteolin, quercetin, stigmasterol, among others.[7]

Chronic consumption of STVR represents little risk based on human studies. In 1985 it was shown that oral consumption of STVR in high amounts as 550 mg/kg of body weight per day (i.e., 200 times the maximum probable intake of around 2 mg/kg/body weight/day for two years) had no toxic or carcinogenic effects in rats. The pharmacological effects are suggested by other studies, such as the reduction of blood pressure and blood glucose levels. The metabolite of aglycone, steviol, was reported to be mutagenic and bactericidal in Salmonella typhimurium TM677. Therefore, the biological effects and adverse drug interactions are confusing.[8]

We publish characteristics, properties and quantum interactions of nitrogenous bases through simulation methods of quantum chemistry.[9-13]

In this work, the general objective was to analyze the chemo-quantum interactions of Steviol and nitrogenous bases.

MATERIALS AND METHODS

Software and simulation

It used HyperChem molecular simulator for Windows Serial # 12-800-1501800080 SE-PM3 for extracting the molecules.

General setting

SE-PM3 a total load of around 0. Multiplicity1. Pairing turns the RHF. State under the Convergent limit of 0.01. 50. Limit iteration accelerates convergence Yes. Polarizability. Geometry Optimization: Algorithms Polak-Ribiere (conjugate gradient). RMS termination condition gradient 0.1 kcal/Amol. Algorithm Polak-Ribiere (conjugate gradient), the termination condition or 1000 cycles Maximum. Algorithm Polak-Ribiere (conjugate gradient).

Parameters for the calculation of molecular orbitals HOMO and LUMO.

Orbitals Plot Orbitals Options Isosurface Rendering. Orbital Contour Value 0.05. Wire Isosurface Gird months. Gird Meshes size Coarse. Gird Layout Default. Gird Contour Default. Transparency Level Default.

Parameters for the calculation of Electrostatic Potential.

Plot Molecular Graphs. Plot Molecuar Options. Molecular Properties: Properties. Electrostatic Potential Yes. Representations 3D Mapped Isosurface. Gird Mesh Size Coarse. Gird Layout Default. Contour Gird Default. Isosurface Reading. Total Charge Density Contour Value 0.015. Rendering Wire Mesh. Transparency Level Default. Mapped Options Functions Default. [14]

RESULTS AND DISCUSSION

Table 1 shows the crossed bands of ETC of the amino acids with STV. In this same table, the interactions of the pure substances are included and compared with the crossed bands. Interaction 1, water: water has the highest ETC of all possible interactions. That tells us that water is the most interactive substance of all. The minimum ETC is presented by the G-G interaction. This ETC represents the most stable interaction.

Table 1: ETC pure substance and, cross-linked strains of amino acids with Steviol.

No.	Reducing Agent	Oxidizing Agent	HOMO	LUMO	BG	E-	E+	EP	ETC
1	Water	Water	-12.316	4.059	16.375	-0.127	0.171	0.298	54.950
2	Water	Steviol	-12.316	0.983	13.299	-0.127	0.117	0.244	54.505
3	Steviol	Water	-9.811	4.059	13.870	-0.136	0.171	0.307	45.179
4	T	Steviol	-9.710	0.983	10.694	-0.124	0.117	0.241	44.373
5	U1	Steviol	-9.710	0.983	10.694	-0.127	0.117	0.244	43.827
6	U2	Steviol	-9.882	0.983	10.865	-0.136	0.117	0.253	42.945
7	Steviol	Steviol	-9.811	0.983	10.794	-0.136	0.117	0.253	42.665
8	C	Steviol	-9.142	0.983	10.126	-0.160	0.117	0.277	36.555
9	G	Steviol	-8.537	0.983	9.520	-0.145	0.117	0.262	36.338
10	A	Steviol	-8.556	0.983	9.539	-0.155	0.117	0.272	35.071
11	Steviol	C	-9.811	-0.344	9.467	-0.136	0.154	0.290	32.646
12	Steviol	A	-9.811	-0.234	9.577	-0.136	0.165	0.301	31.816
13	T	T	-9.710	-0.511	9.200	-0.124	0.172	0.296	31.080
14	Steviol	G	-9.811	-0.206	9.605	-0.136	0.176	0.312	30.785
15	U1	U1	-9.710	-0.511	9.200	-0.127	0.176	0.303	30.362
16	Steviol	T	-9.811	-0.511	9.300	-0.136	0.172	0.308	30.195
17	Steviol	U1	-9.811	-0.511	9.300	-0.136	0.176	0.312	29.808
18	U2	U2	-9.882	-0.428	9.454	-0.136	0.189	0.325	29.090
19	*Steviol*	*U2*	*-9.811*	*-0.428*	*9.383*	*-0.136*	*0.189*	*0.325*	*28.872*
20	C	C	-9.142	-0.344	8.799	-0.160	0.154	0.314	28.021
21	A	A	-8.556	-0.234	8.322	-0.155	0.165	0.320	26.005
22	G	G	-8.537	-0.206	8.331	-0.145	0.176	0.321	25.953

Solubility of commercials stevia vs. steviol in water

The Steviol-Water interaction has a lower ETC (Figure 1). Steviol has a medium solubility, due to its low ETC when combined with water.

In this figure, the red dashed line represents the lower limit, that is, the ETC value of steviol. The green dotted line represents the upper limit, that is, the water ETC value. The blue dot represents the bottom of the quantum well of the Water:Steviol interaction. While the green dot represents the bottom of the quantum well and the ETC value of the Steviol:Water interaction.

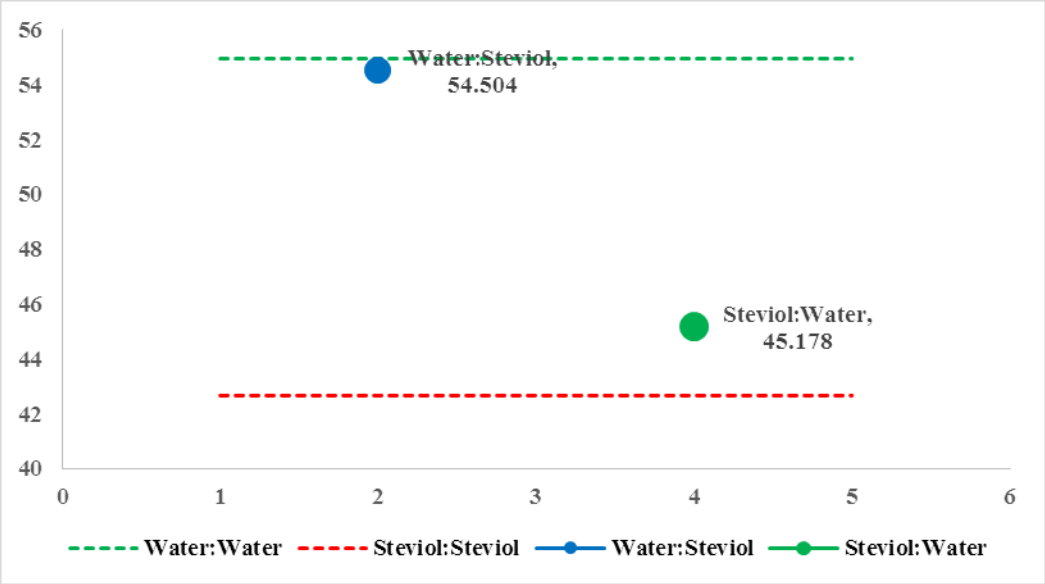

Figure 1: Electron transfer coefficient (quantum well) Steviol: Water.

Above the red line, the zone with the lowest probability of some interaction between these two compounds is located. Below the red line is the area most likely to have an electron transfer interaction between these two compounds. Between the two lines, there is the zone of average probability of the interaction between these two compounds.

Table 2: Experimental parameters and solubility; * slightly soluble ** moderately soluble * completely soluble; V: Steviol, W: Commercial Sweeny; M: Commercial Mayan Sweet.**

Sample	Temperature (^{o}C)	Agitation (rpm)	Dilution time (seg)	Solubility
V	25	500	60	**
W	25	500	10	***
M	25	500	350	*
V	35	500	60	**
W	35	500	5	***
M	35	500	350	*
V	65	500	10	**
W	65	500	5	***
M	65	500	350	*

We perform Steviol solubility tests and commercial stevia in water at different temperatures (table 2, fig. 2). The results showed the median solubility for steviol as predicted by the theoretical calculations in Table 1. Although several parameters were changed, steviol remained at its median solubility.

The commercial stevia showed different solubilities. These differences show us that commercial stevia has other compounds than steviol.

As expected, steviol diluted faster with increasing temperature (Chatelier principle), but it retained its medium solubility in water.

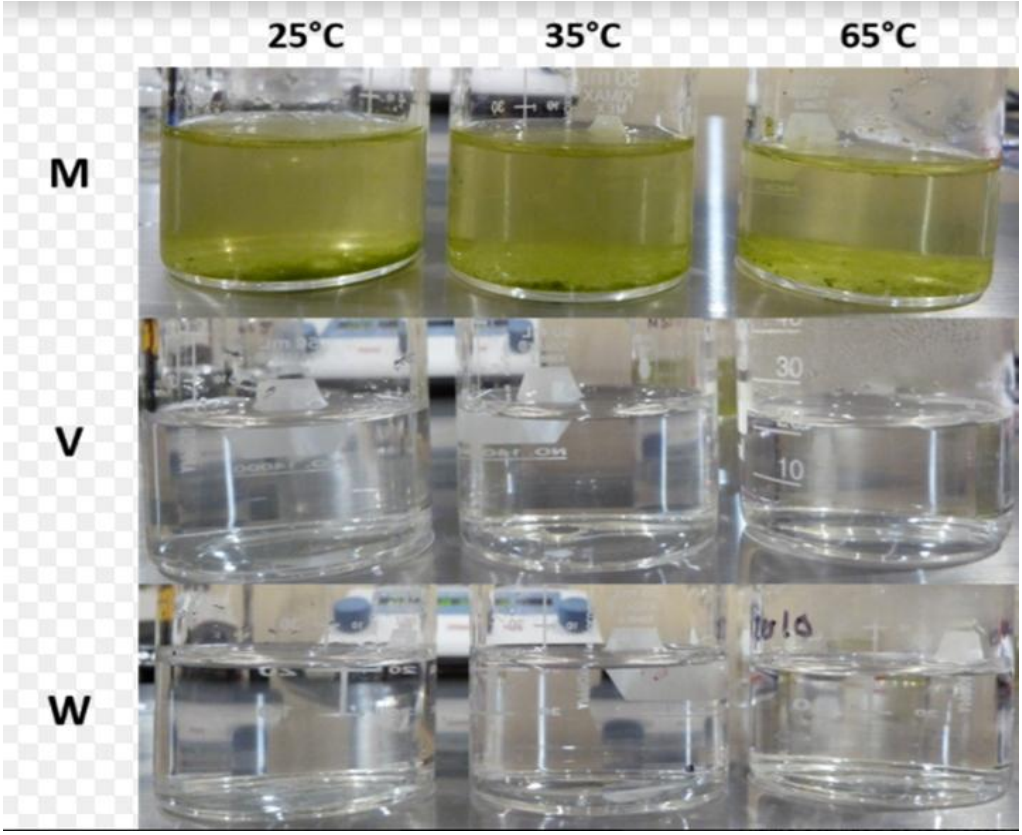

Figure 2: Solubility tests of Steviol and Water.

Interactions of Steviol vs. Nitrogen Bases (DNA, RNA)

The lowest interaction of Steviol:U2 is ETC =28,872 (Table 1). The high probability that Steviol causes a mutation in RNA due to its interaction with U2 is shown.

The epistemology of figure 3 it is similar to figure 1. In this figure, we can see that the Steviol: U2 interaction is the smallest of all crossed-bands of table 1. Therefore, steviol interacts better with U2 and this situation can cause alterations in the RNA. This alteration is similar to that caused by nicotine to RNA as well.[15]

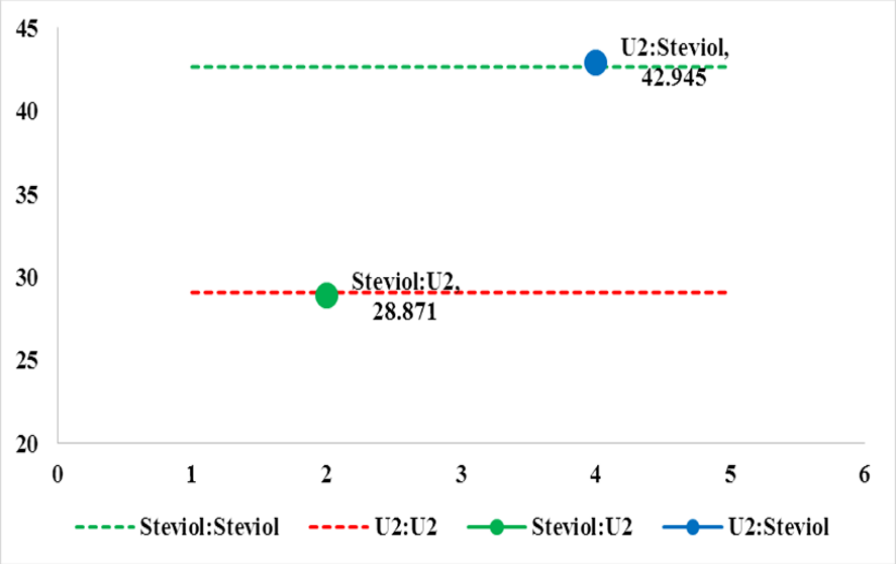

Figure 3: Electron transfer coefficient (quantum well) Steviol: Water.

Another important observation is that Steviol acts as a reducing agent (antioxidant) in all nitrogenous bases; but, it is not reliable; for its low cross-band ETC with U2.

CONCLUSION

Therefore, we conclude that not all antioxidant substances are good for health.

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