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RESEARCH CARCINOGENIC EFFECT OF TARTRAZINE VS NITROGENOUS BASES BY THE QUANTUM METHOD (ZINDO/ 1).

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ABSTRACT

Tartrazine yellow dye whose structure tine trisodium salt of 3-carboxy-5-hydroxy benzene pyrazolone-1 (p-sulfophenyl) - 4 - (sulfophenyl azo). Azo dyes have a group (-N = N-) in its chemical structure. In this research, the carcinogenic effect of tartrazine vs. nitrogenous bases by quantum method (Zindo/1) was determined. The simulations realized with molecular simulator Hyper Chem (HC). The specific parameters selected for each of the simulations were calculated by Semi-Empirical Method: ZINDO/1. Tartrazine has the lowest of all substances ETC because of its small ETC is the most chemically stable material. Interaction Guanine-Tartrazine has the lowest ETC 10.8431373, therefore, is most likely the interaction between compounds.

KEYWORDS: Tartrazine, Cancer, Nitrogenous bases, Quantum method.

INTRODUCTION

Tartrazine yellow dye whose structure tine trisodium salt of 3-carboxy-5-hydroxy benzene pyrazolone-1 (p-sulfophenyl) - 4 - (sulfophenyl azo)[1]. Azo dyes have a group (-N = N-) in its chemical structure[2]. Tartrazine is an artificial azo dye used in food, pharmaceuticals[3] dyes, cosmetics,[1] dairy products, cereals[4], instant noodles, soft drinks and biscuits[5]. Tartrazine has to be controlled in food commodities due their potential harmfulness to

humans according to the European Union [EU] and the Federal Food, cosmetics[6]. The allowable level of synthetic food colors in the mixing ratio is 100 ppm[7]. The tartrazine intake can cause a variety of side-effects[8].

Tartrazine cause damage to organs biochemical markers[9] at different doses[8] causes diseases: such as hyperactivity, asthma[10]. Mpountoukas et al. They showed that tartrazine has a high potential genotoxic in human lymphocytes. Tartrazine binds directly to DNA[11]. Kashanian et al. They also reported similar results and said tartrazine was potentially toxic to DNA in vitro calf thymus[12]. Li et al. reported the toxic interaction between tartrazine and bovine hemoglobin (BHB), it was found to have a toxic effect tartrazine[13]. Animal studies have also established the DNA damaging effects (mutagenic) Tartrazine[14].

Recent publications show that the metabolites of tartrazine, are carcinogenic[1]. Tartrazine produces thyroid cancer[15]. Cancer is related to food, nutrition and physical activity in high-income countries[16]. Carcinogens are through food[17]. Cancer is one of the leading causes of death worldwide[18].

In previous publications disclosed the results of ETC and possible combinations of NB 36 that make up DNA and RNA The difference between the ETC of the 36 possible combinations of 6 NB is 10,620. The difference between the cross and allowed bands is only 2.38 (Table 2). Because of this small difference, mutations are carried out very easily, are not compatible with 88.88% of these combinations. Enzymes have a great job cleaning[19-22].

Computational methods in quantum chemistry are responsible for identifying more stable molecular systems, and make definite predictions[23]. Fragments or molecular structural designs (or other waste) provide detailed maps of chemical, biological interactions[24].

The surfaces of the interaction of DNA[25] and the proteins identified using a computer[26-27]. In particular, the theoretical vibrational frequencies and geometric parameters (bond lengths and bond angles) can be calculated using ab initio Hartree-Fock (HF)[28]. In this research, the carcinogenic effect of tartrazine VS nitrogenous bases by quantum method (Zindo/1) was determined.

METHODOLOGY

a. Abbreviations

Highest Occupied Molecular Orbital (HOMO). Lowest Unoccupied Molecular Orbital (LUMO). Band Gap (BG), Negative Energy (E-). Positive Energy (E+). Electrostatic Potential (EP). Electronic Transfer Coefficient (ETC). Uracil Tautomer 1 (UT1). Uracil Tautomer 2 (UT2) Figure 1.

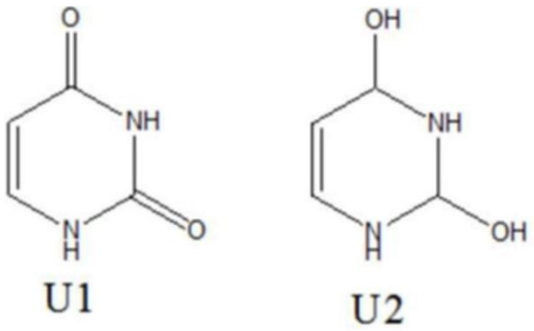

Fig. 1 Tautomers of U. U tautomer U T1 has ketone links. U tautomer U T2 has hydroxyl links. Sorce [19].

b. Computational method

The simulations realized with molecular simulator Hyper Chem (HC). (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)[20].

The computational model used was; HC Semi-Empirical Parameterized Model number 3 (SE- Zindo/1) to draw the corresponding molecules. These were then processed using SE-PM3.The geometry realized with the Polak Ribiere method. The computational quantum chemistry variables calculated: HOMO-LUMO, BG, EP and other properties, resulting in a delimited table tab for BG and EP[20].

The specific parameters selected for each of the simulations were as follows: SET UP[20]. Semi-Empirical Method: ZINDO/1. Semi-Empirical Options: Charge and Spin. Total Charge 0. Spin Multiplicity 1. SCF Control. Converge limit 0.01. Interaction limit 1000. Accelerate converge Yes. Spin Pairing Lowest. Overlap Weighting Factors Sigma-Sigma 1, Pi-Pi 1. Polarizabilities do not calculate.

Computation 1. Geometry Optimization. Algorithm Polak Ribiere (conjugate gradient). Options Termination conditions. RMS gradient of 0.1 kcal/mol or 1000 maximum cycles. In vacuo yes. Screen refresh period one cycles.

Computation 2. Orbitals. Plot Orbital Options Isosurface Rendering. Orbital Contour Value 0.05. Rendering Wire meshes Isosurface Grid. Grid meshes size Coarse. Grid layout Default. Gird contour Default. Transparency level Default.

Computation 3. Plot Molecular Graphs. Plot Molecular Options. Molecular Properties. Properties. Electrostatic Potential Yes. Representations. 3D Mapped Isosurface. Grid Mesh Size Coarse. Grid layout Default. Contour gird Default. Isosurface Rereading. Total Charge Density Contour Value (TCDCV) 0.015. Rendering Wire meshes. Transparency level Default. Mapped Options Functions Default[19, 20].

c. Formulas

The calculations obtained correspond to the theory ETC[20].This method is calculating the ratio of dividing the BG / EP. This ratio indicates the multiples of the EP that the electron jumps its BG.

$$ETC = \left|\frac{BG}{EP}\right| \quad (1)$$

The EP is equal to the absolute value of the difference (E+) – (E-).

$$EP = |E + -E -| \quad (2)$$

The BG is equal to the absolute value of the difference (HOMO) – (LUMO) [20-22].

$$BG = |HOMO - LUMO| \quad (3)$$

Table 1: The combination of tartrazine ETC bases and nitrogen

CHEMICAL SUBSTANCE	HOMO	LUMO	BG	E-	E+	EP	ETC
TARTRAZINE	-6.946	0.251	7.197	-0.202	0.361	0.563	12.783
GUANINE	-5.832	7.303	13.135	-0.200	0.181	0.381	34.475
CYTOSINE	-6.947	6.340	13.287	-0.211	0.166	0.377	35.244
TIMINA	-7.651	6.051	13.702	-0.168	0.169	0.337	40.659
URACIL T1	-8.324	5.976	14.300	-0.168	0.178	0.346	41.329
URACIL T2	-8.506	6.838	15.344	-0.147	0.215	0.362	42.387
ADENINE	-5.757	7.745	13.502	-0.138	0.174	0.312	43.276

The table shows the tartrazine interactions vs. nitrogenous bases. It also lists the results of ETC substances químicas. Tartrazine has the lowest of all substances ETC. Tartrazine because of its small ETC is the most chemically stable material. Adenine has ETC very high. Therefore, it is chemically unstable according to the results.

Table 2. Crossband dye (tartrazine) purine and pyrimidine bases

CHEMICAL SUBSTANCE		HOMO	LUMO	BG	E-	E+	EP	ETC
GUANINE	TARTRAZINE	-5.832	0.251	6.083	-0.200	0.361	0.561	10.843
ADENINE	TARTRAZINE	-5.757	0.251	6.008	-0.138	0.361	0.499	12.040
CYTOSINE	TARTRAZINE	-6.947	0.251	7.198	-0.211	0.361	0.572	12.584
TARTRAZINE	TARTRAZINE	-6.946	0.251	7.197	-0.202	0.361	0.563	12.783
TARTRAZINE	TARTRAZINE	-6.946	0.251	7.197	-0.202	0.361	0.563	12.783
TIMINA	TARTRAZINE	-7.651	0.251	7.902	-0.168	0.361	0.529	14.938
URACIL T1	TARTRAZINE	-8.324	0.251	8.575	-0.168	0.361	0.529	16.210
URACIL T2	TARTRAZINE	-8.506	0.251	8.757	-0.147	0.361	0.508	17.238
TARTRAZINE	URACIL T2	-6.946	6.838	13.784	-0.202	0.215	0.417	33.055
TARTRAZINE	URACIL T1	-6.946	5.976	12.922	-0.202	0.178	0.380	34.005
TARTRAZINE	TIMINA	-6.946	6.051	12.997	-0.202	0.169	0.371	35.032
TARTRAZINE	CYTOSINE	-6.946	6.340	13.286	-0.202	0.166	0.368	36.103
TARTRAZINE	GUANIE	-6.946	7.303	14.249	-0.202	0.181	0.383	37.204
TARTRAZINE	ADENINE	-6.946	7.745	14.691	-0.202	0.174	0.376	39.072

The table shows the results of the interaction, tartrazine LUMO and HOMO vs. nitrogenous bases of DNA and RNA. Interaction Guanine-Tartrazine has the lowest ETC = 10.843, therefore, is most likely the interaction between compounds. Tartrazine- Adenine has a 39.072 ETC is the highest according to the data.

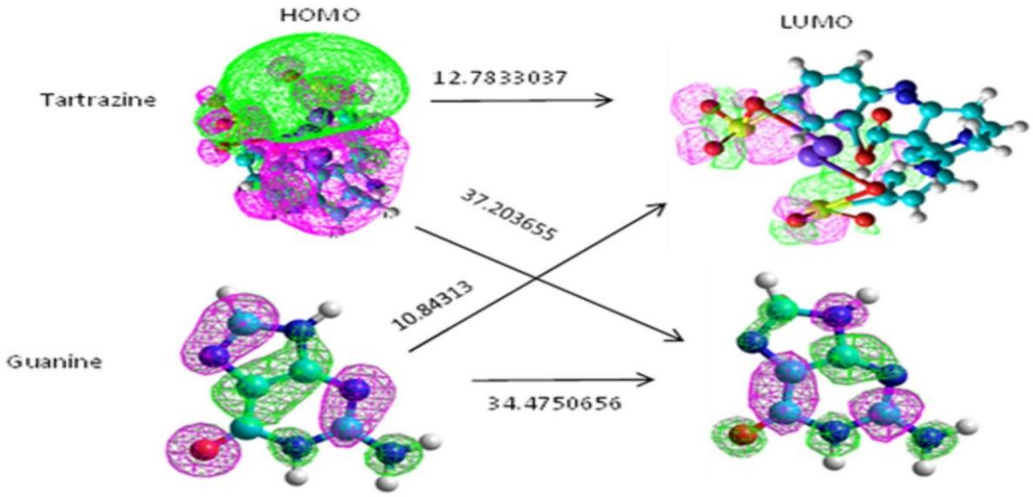

Fig. 2: in this figure, the number of the smallest value for all bands of guanine interactions tartrazine (10.843) is shown.

CONCLUSION

The research provides enough evidence by quantum chemistry methods. Tartrazine may be bonded directly with guanine. The results of the cross bands reveal that ETC. Therefore, interaction Adenine-Tartrazine is more stable. Research shows that if affects human DNA and RNA. The results are similar to those described in other investigations. The scientific contribution of this paper is the point of interaction of Tartrazine, and the nearest ETCs With the nitrogenous bases. Due to the small differences in the ETCs possible combinations of the Tartrazine with nitrogenous bases, interactions are highly likely to harm both DNA and RNA This research provides new options for the study on the carcinogenicity of tartrazine.

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