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QUANTUM CHEMICAL ANALYSIS OF ETHANOL AND ITS INTERACTION WITH AMINO ACIDS AND DIPEPTIDES (CARNOSINE)

Nadia Limón Olmos[1], Carolina del Carmen Pérez Sánchez[2], Marcos Alberto Ramírez Perez[3], Temani Duran Mendoza[2], Maria Concepcion de la Cruz Leyva[2], Verónica Rodríguez Soria[4], Laura Contreras Mioni[4] and Manuel González Perez*[5, 6]

[1]Universidad Popular Autónoma del Estado de Puebla (UPAEP). Facultad de Medicina. (Servicio de Beca).

[2]Universidad Juárez Autónoma de Tabasco (UJAT). División Académica Multidisciplinaria de los Ríos (DAMR).

[3]Universidad Autónoma de Yucatán. Facultad de Medicina (Residente).

[4]UPAEP. Decanato de Ciencias Biológicas.

[5]UPAEP. Posgrado en Ciencias de la Ingeniería Biomédica.

[6]Sistema Nacional de Investigadores. Nivel 1.

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***Corresponding Author**
Manuel González Perez
UPAEP. Posgrado en Ciencias de la Ingeniería Biomédica.

ABSTRACT

Ethanol (EtOH) is a product highly consumed today; it is part of the daily life of the majority of the people. The objective of this investigation was to calculate the quantum interactions between EtOH, Amino Acids (AAs), and dipeptides of AAs. In particular, carnosine. The Hyperchem software and the Electron Transfer Coefficient (ETC) theory were used. As single substances in crossed bands, we found that the EtOH percentage works best as an antioxidant in 88.89% of all these possible interactions. As dipeptides, we made 800 interactive calculations with the EtOH molecule; we found that of the 800 interactions 260 (32.5%) are oxidants with high and medium probability and 540 (67.5%) are not oxidants. As a particular case, EtOH oxidizes carnosine. We conclude excess EtOH molecules can destroy the carnosine. We recommend that children, young people, and sports people should not ingest alcohol because it can damage its carnosine. Our calculations coincide with the medical literature and the Mediterranean diet.

KEYWORDS: Ethanol, Amino Acids, Quantum Chemical, Carnosine, Dipeptides.

INTRODUCTION

EtOH is oxidized to acetaldehyde within the hepatocyte; using three metabolic routes: A) in the cytosol by the enzyme alcohol dehydrogenase (ADH). B) In the endoplasmic reticulum by cytochrome P450 (CYP2E1). C) In the peroxisomes by the catalase enzyme. The metabolic consequences of oxidation by ethanol include an alteration of cytoplasmic and mitochondrial redox. These metabolic consequences generate high free radicals derived from the production of oxygen and nitrogen. The metabolic pathway is located in the respiratory chain of the mitochondria.[1-10]

DNA is a substance that is characterized by containing the genetic information of each one and transmitting it to their descendants. This genetic substance is a polynucleotide composed of deoxyribose (sugar), nitrogenous bases and a phosphate group. RNA (ribonucleic acid) has a similar composition (ribose, nitrogenous bases, and phosphate). Its primary function is to transmit the information of the DNA to the cells to generate proteins. In addition, the ARM carries out catalytic processes. Both substances are indispensable for the proper functioning of living human beings. At the moment of altering the nitrogen bases, either DNA or RNA, irreversible effects are generated that can lead to permanent and irreparable damage to the structures of an organism.[11,12]

Within the human body, when alcohol interacts with bases according to recent research, different levels of affectation were found. These levels are genotoxicity and teratogenicity.[13]

Other researchers found that alcohol adversely affects intrauterine pregnancy in the human fetus. As part of this affliction, a nervous syndrome known as the fetus -alcoholic and[14] effects of the fetal alcohol syndrome- is triggered. It was also found that there are critical periods in life where alcohol consumption can lead to banking brain loss. This loss has its genesis from processes of myelination, neuroinflammation, brain damage[15] and epigenetic changes.

On the other hand, some researchers inform us that a new carnosine derivative resistant to bioavailable carnosinase prevents the onset and stops the progression of diabetic nephropathy in mice.[16] Also, carnosine supplementation improves serum resins concentrations in sedentary adults who are overweight or obese.[17]

The objective of this investigation was to calculate the quantum interactions between EtOH, AAs, and dipeptides of AAs. In particular, carnosine.

MATERIALS AND METHODS

The Hyperchem software and the ETC electron transfer coefficient theory were used. In these calculations, the quantum parameters reported in previous publications were taken.[18-25]

RESULTS AN DISCUSSION

Pure substances

In table 1. We can see that EtOH has the highest ETC as a pure substance; due to its high ETC, it can attack all essential AAs. On the other hand, the Arg presents the lowest ETC of all the substances in question; therefore, due to its lower ETC Arg is the most stable of all AAs.

Table 1: Calculation of ETCs of pure substances plus EtOH.

No.	Reducing Agent	Oxidizing Agent	HOMO	LUMO	BG	E-	E+	EP	ETC
1	EtOH	EtOH	-10.898	3.334	14.232	-0.119	0.151	0.270	52.711
2	Val	Val	-9.914	0.931	10.845	-0.131	0.109	0.240	45.188
3	Ala	Ala	-9.879	0.749	10.628	-0.124	0.132	0.256	41.515
4	Leu	Leu	-9.645	0.922	10.567	-0.126	0.130	0.256	41.279
5	Phe	Phe	-9.553	0.283	9.836	-0.126	0.127	0.253	38.879
6	Gly	Gly	-9.902	0.902	10.804	-0.137	0.159	0.296	36.500
7	Ser	Ser	-10.156	0.565	10.721	-0.108	0.198	0.306	35.037
8	Cys	Cys	-9.639	-0.236	9.403	-0.129	0.140	0.269	34.956
9	Glu	Glu	-10.374	0.438	10.812	-0.111	0.201	0.312	34.655
10	Ile	Ile	-9.872	0.972	10.844	-0.128	0.188	0.316	34.316
11	Thr	Thr	-9.896	0.832	10.728	-0.123	0.191	0.314	34.167
12	Gln	Gln	-10.023	0.755	10.778	-0.124	0.192	0.316	34.108
13	Asp	Asp	-10.370	0.420	10.790	-0.118	0.204	0.322	33.509
14	Asn	Asn	-9.929	0.644	10.573	-0.125	0.193	0.318	33.249
15	Lys	Lys	-9.521	0.943	10.463	-0.127	0.195	0.322	32.495
16	Pro	Pro	-9.447	0.792	10.238	-0.128	0.191	0.319	32.095
17	Trp	Trp	-8.299	0.133	8.431	-0.112	0.155	0.267	31.577
18	Tyr	Tyr	-9.056	0.293	9.349	-0.123	0.193	0.316	29.584
19	His	His	-9.307	0.503	9.811	-0.169	0.171	0.340	28.855
20	Met	Met	-9.062	0.145	9.207	-0.134	0.192	0.326	28.243
21	Arg	Arg	-9.176	0.558	9.734	-0.165	0.199	0.364	26.742

Chemical stability increases as the ETC decreases. The chemical reactivity increases as the ETC of each substance increases. These observations are in accordance with the depth theory of quantum wells.

Substances in crossed bands

The crossed bands consist of taking the value of the HOMO energy of one substance and amount it of the LUMO of another substance. The operation for E- and E + of the electrostatic potential is similar.

The ETC of crossed bands is the quotient of dividing the absolute value of the difference between HOMO and LUMO (band gap) between the absolute value of the difference between E- and E + of the electrostatic potential.

Table 2: Calculation of ETCs of substances in crossed bands.

No.	Reducing Agent	Oxidizing Agent	HOMO	LUMO	BG	E-	E+	EP	ETC
1	EtOH	EtOH	-10.898	3.334	14.232	-0.119	0.151	0.270	52.711
2	Glu	EtOH	-10.374	3.334	13.708	-0.111	0.151	0.262	52.320
3	Ser	EtOH	-10.156	3.334	13.490	-0.108	0.151	0.259	52.085
4	EtOH	Val	-10.898	0.931	11.829	-0.119	0.109	0.228	51.883
5	Asp	EtOH	-10.370	3.334	13.704	-0.118	0.151	0.269	50.943
6	Gln	EtOH	-10.023	3.334	13.357	-0.124	0.151	0.275	48.570
7	Thr	EtOH	-9.896	3.334	13.230	-0.123	0.151	0.274	48.285
8	Asn	EtOH	-9.929	3.334	13.263	-0.125	0.151	0.276	48.054
9	Ala	EtOH	-9.879	3.334	13.212	-0.124	0.151	0.275	48.045
10	EtOH	Leu	-10.898	0.922	11.820	-0.119	0.130	0.249	47.471
11	Ile	EtOH	-9.872	3.334	13.206	-0.128	0.151	0.279	47.333
12	Val	EtOH	-9.914	3.334	13.248	-0.131	0.151	0.282	46.977
13	Leu	EtOH	-9.645	3.334	12.979	-0.126	0.151	0.277	46.856
14	Phe	EtOH	-9.553	3.334	12.887	-0.126	0.151	0.277	46.523
15	EtOH	Ala	-10.898	0.749	11.647	-0.119	0.132	0.251	46.404
16	Cys	EtOH	-9.639	3.334	12.972	-0.129	0.151	0.280	46.330
17	Lys	EtOH	-9.521	3.334	12.854	-0.127	0.151	0.278	46.239
18	Gly	EtOH	-9.902	3.334	13.236	-0.137	0.151	0.288	45.959
19	Pro	EtOH	-9.447	3.334	12.780	-0.128	0.151	0.279	45.807
20	EtOH	Phe	-10.898	0.283	11.182	-0.119	0.127	0.246	45.453
21	Tyr	EtOH	-9.056	3.334	12.390	-0.123	0.151	0.274	45.218
22	Trp	EtOH	-8.299	3.334	11.632	-0.112	0.151	0.263	44.229
23	Met	EtOH	-9.062	3.334	12.396	-0.134	0.151	0.285	43.494
24	EtOH	Gly	-10.898	0.902	11.800	-0.119	0.159	0.278	42.445
25	EtOH	Cys	-10.898	-0.236	10.663	-0.119	0.140	0.259	41.169
26	EtOH	Trp	-10.898	0.133	11.031	-0.119	0.155	0.274	40.258
27	Arg	EtOH	-9.176	3.334	12.510	-0.165	0.151	0.316	39.588
28	His	EtOH	-9.307	3.334	12.641	-0.169	0.151	0.320	39.504
29	EtOH	His	-10.898	0.503	11.401	-0.119	0.171	0.290	39.315
30	EtOH	Ile	-10.898	0.972	11.870	-0.119	0.188	0.307	38.664
31	EtOH	Thr	-10.898	0.832	11.730	-0.119	0.191	0.310	37.839
32	EtOH	Pro	-10.898	0.792	11.690	-0.119	0.191	0.310	37.710
33	EtOH	Lys	-10.898	0.943	11.841	-0.119	0.195	0.314	37.710

34	EtOH	Gln	-10.898	0.755	11.653	-0.119	0.192	0.311	37.470
35	EtOH	Asn	-10.898	0.644	11.542	-0.119	0.193	0.312	36.995
36	EtOH	Ser	-10.898	0.565	11.463	-0.119	0.198	0.317	36.161
37	EtOH	Arg	-10.898	0.558	11.456	-0.119	0.199	0.318	36.026
38	EtOH	Tyr	-10.898	0.293	11.191	-0.119	0.193	0.312	35.868
39	EtOH	Met	-10.898	0.145	11.043	-0.119	0.192	0.311	35.509
40	EtOH	Glu	-10.898	0.438	11.337	-0.119	0.201	0.320	35.427
41	EtOH	Asp	-10.898	0.420	11.318	-0.119	0.204	0.323	35.041

In Table 2, the calculations of the crossed bands of EtOH with each of the AA are shown. The results are fascinating.

Other impressive results are the calculations of the probability of agreement in the quantum wells (fig.1).

In figure 1, the dashed lines represent the limits ETCs of the pure substances.

The zone most likely to occur is the lowest area. The middle region is located in the middle of the two broken lines. The territory of low occurrence of quantum interactions is situated above the broken line of higher ETC.

In this figure 1. An extreme case of oxidation of EtOH is presented. The red dot represents the oxidation of EtOH to Val. The green dot represents the anti-oxidation of EtOH to Val. It can be seen that both are located in the zone of the average probability of occurrence. Even within the region of average probability of occurrence the red point is the deepest, therefore it is of higher presence of the two possibilities.

Even so, only 11.11% of the interactions of EtOH with AAs are oxidative. The rest are antioxidants with medium to high probabilities.

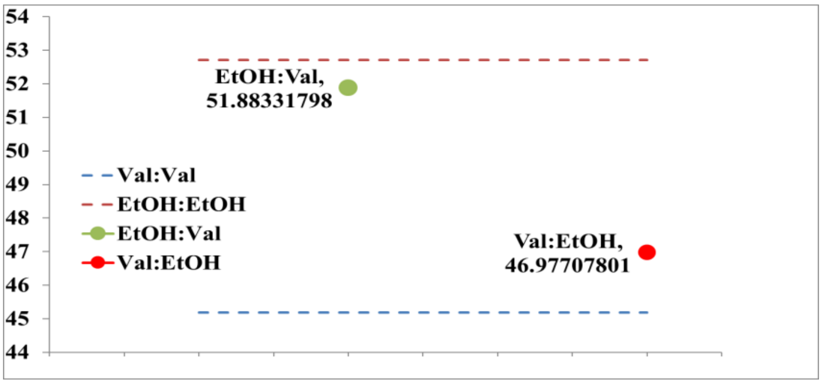

Figure 1: Quantum well of the Val: EtOH interaction. It can be seen that EtOH has a lower ETC when it acts as an oxidizing agent. This interaction falls in the average probability zone.

The Val: EtOH interaction has a lower ETC when the EtOH behaves as an oxidizing agent. Nevertheless, due to this interaction, EtOH can cause health problems by oxidizing Val. This.

Table 2: Calculation of ETCs interactions EtOH: dipeptides integrated to proteín Etoh.

No.	Reducing Agent	Oxidizing Agent	HOMO	LUMO	BG	E-	E+	EP	ETC
501	Arg:Val	EtOH:EtOH	-9.176	3.334	12.510	-0.165	0.151	0.316	39.588
502	Arg:Leu	EtOH:EtOH	-9.176	3.334	12.510	-0.165	0.151	0.316	39.588
503	Arg:Ala	EtOH:EtOH	-9.176	3.334	12.510	-0.165	0.151	0.316	39.588
504	Arg:Phe	EtOH:EtOH	-9.176	3.334	12.510	-0.165	0.151	0.316	39.588
505	Arg:Gly	EtOH:EtOH	-9.176	3.334	12.510	-0.165	0.151	0.316	39.588
506	Arg:Cys	EtOH:EtOH	-9.176	3.334	12.510	-0.165	0.151	0.316	39.588
507	Arg:Trp	EtOH:EtOH	-9.176	3.334	12.510	-0.165	0.151	0.316	39.588
508	Arg:His	EtOH:EtOH	-9.176	3.334	12.510	-0.165	0.151	0.316	39.588
509	Arg:Ile	EtOH:EtOH	-9.176	3.334	12.510	-0.165	0.151	0.316	39.588
510	Arg:Thr	EtOH:EtOH	-9.176	3.334	12.510	-0.165	0.151	0.316	39.588
511	Arg:Lys	EtOH:EtOH	-9.176	3.334	12.510	-0.165	0.151	0.316	39.588
512	Arg:Pro	EtOH:EtOH	-9.176	3.334	12.510	-0.165	0.151	0.316	39.588
513	Arg:Gln	EtOH:EtOH	-9.176	3.334	12.510	-0.165	0.151	0.316	39.588
514	Arg:Asn	EtOH:EtOH	-9.176	3.334	12.510	-0.165	0.151	0.316	39.588
515	Arg:Ser	EtOH:EtOH	-9.176	3.334	12.510	-0.165	0.151	0.316	39.588
516	Arg:Arg	EtOH:EtOH	-9.176	3.334	12.510	-0.165	0.151	0.316	39.588
517	Arg:Tyr	EtOH:EtOH	-9.176	3.334	12.510	-0.165	0.151	0.316	39.588
518	Arg:Glu	EtOH:EtOH	-9.176	3.334	12.510	-0.165	0.151	0.316	39.588
519	Arg:Met	EtOH:EtOH	-9.176	3.334	12.510	-0.165	0.151	0.316	39.588
520	Arg:Asp	EtOH:EtOH	-9.176	3.334	12.510	-0.165	0.151	0.316	39.588
521	His:Val	EtOH:EtOH	-9.307	3.334	12.641	-0.169	0.151	0.320	39.504
522	His:Leu	EtOH:EtOH	-9.307	3.334	12.641	-0.169	0.151	0.320	39.504
523	*His:Ala	EtOH:EtOH	-9.307	3.334	12.641	-0.169	0.151	0.320	39.504
524	His:Phe	EtOH:EtOH	-9.307	3.334	12.641	-0.169	0.151	0.320	39.504
525	His:Gly	EtOH:EtOH	-9.307	3.334	12.641	-0.169	0.151	0.320	39.504
526	His:Cys	EtOH:EtOH	-9.307	3.334	12.641	-0.169	0.151	0.320	39.504
527	His:Trp	EtOH:EtOH	-9.307	3.334	12.641	-0.169	0.151	0.320	39.504
528	His:His	EtOH:EtOH	-9.307	3.334	12.641	-0.169	0.151	0.320	39.504
529	His:Ile	EtOH:EtOH	-9.307	3.334	12.641	-0.169	0.151	0.320	39.504
530	His:Thr	EtOH:EtOH	-9.307	3.334	12.641	-0.169	0.151	0.320	39.504
531	His:Lys	EtOH:EtOH	-9.307	3.334	12.641	-0.169	0.151	0.320	39.504
532	His:Pro	EtOH:EtOH	-9.307	3.334	12.641	-0.169	0.151	0.320	39.504
533	His:Gln	EtOH:EtOH	-9.307	3.334	12.641	-0.169	0.151	0.320	39.504
534	His:Asn	EtOH:EtOH	-9.307	3.334	12.641	-0.169	0.151	0.320	39.504
535	His:Ser	EtOH:EtOH	-9.307	3.334	12.641	-0.169	0.151	0.320	39.504
536	His:Arg	EtOH:EtOH	-9.307	3.334	12.641	-0.169	0.151	0.320	39.504
537	His:Tyr	EtOH:EtOH	-9.307	3.334	12.641	-0.169	0.151	0.320	39.504
538	His:Glu	EtOH:EtOH	-9.307	3.334	12.641	-0.169	0.151	0.320	39.504
539	His:Met	EtOH:EtOH	-9.307	3.334	12.641	-0.169	0.151	0.320	39.504
540	His:Asp	EtOH:EtOH	-9.307	3.334	12.641	-0.169	0.151	0.320	39.504

**Carnosine*

AA forms an integral part of the muscular tissue and enables the positive nitrogen balance; also, it intervenes in the repair of tissues. The lack of Val generates the genetic disease sickle cell anemia. It is read in the medical literature.

Dipeptides in crossed bands with EtOH

Eight hundred of di-peptide-EtOH interactions were made. These dipeptides were considered bound in proteins.

Table 2 shows the oxidation interactions of the dipeptides. EtOH behaves as an oxidizing agent in 40 interactions (501-541) of the general table of 800 interactions. These interactions are the most likely to damage the proteins of tissues and enzymes.

It can be observed in this table that all dipeptides formed by His and Arg are oxidized with EtOH.

A significant finding is that the interactions from 541 to 800 are the most likely to be carried out due to their lower ETCs (35,041-39,315). In these 260 interactions, EtOH behaves as a reducing or antioxidant agent. This finding confirms the benefits of the Mediterranean diet.

CONCLUSIONS

We made three types of calculations to study the interactions of the EtOH molecule with each of the AAs.

1. As pure substances, we find that EtOH has a higher ETC of all. Due to this lower value of ETC, we conclude that EtOH can interact with any AA in pure form.
2. As single substances in crossed bands. We found that the EtOH percentage works best as an antioxidant in 88.89% of all these interactions.
3. As dipeptides, we made 800 interactive calculations with the EtOH molecule. We found that of the 800 interactions 260 (32.5%) are oxidants with high and medium probability and 540 (67.5%) are not oxidants.
4. As a particular case, EtOH oxidizes carnosine. We conclude excess EtOH molecules can destroy that carnosine.

In general, we conclude that drinking alcohol in small amounts can be useful for the adult's health.

In large quantities, it can produce many health problems because it interacts with the Val and 260 dipeptides of His and Arg as an oxidizing agent.

We recommend that children, young people, and sports people should not ingest alcohol because it can damage carnosine.

Our calculations coincide with the medical literature and the Mediterranean diet.

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