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ANALYSIS OF THE CHEMICAL-QUANTUM INTERACTIONS OF SOME COMPONENTS OF CARROTS VERSUS SARS-COV-2 PROTEINS AND THEIR INFLUENCE ON COVID-19

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ABSTRACT

These days when the COVID-19 pandemic hits the world, it is interesting to study its relationship with nutrition. The carrot is a vegetable consumed around the world. Among its main components is Retinol RTN. These components has notable interactions with the amino acids that make up the SARS-CoV-2 coronavirus that causes the COVID-19 disease. HyperChem molecular modeling software is the tool of choice for the calculations in this work. The electron transfer coefficients (ETC) between the carrot's main components and the amino acids (AA) of the virus are calculated. The interaction of RTN with these AA turns out to be the most stable. Biotin, Vitamin K, and β-carotene are analyzed in the same way. It is concluded that the chemical-quantum interaction of these main carrot components with the AA of the SARS-CoV-2 virus is significantly stable. This conclusion may indicate a recommendation to increase carrot consumption to mitigate the effects of COVID-19.

INTRODUCTION

One of the most popular vegetables grown around the world is the carrot (Daucus Carota). It is one of the primary sources of carotenoids. Carrots are recognized for having various medicinal properties such as antidiarrheal, revitalizing, and diuretic. They are also popularly given the ability to promote good vision.[1-5]

Studies carried out indicate that Daucus Carota is a vital source of vitamin A in the first place and vitamin C in second place.[4-6] It is also a source of energy and fiber for digestion. Calcium is also present and β-carotene as an immune system enhancer.[7]

SARS-CoV-2 causes COVID-19 disease, the pandemic that hits the world this year 2020. This virus is of the RNA type with 30,000 nucleotides in four genes.[8]

There is written evidence in Europe that indicates that carrots were cultivated since before the 10th century. At first, they were used for medicinal purposes, and gradually they were used as food. The first crops were yellow and purple carrots. The orange ones were developed in central Europe in the 15th century and are currently the best known and most used. [7, 9] The popularity of this vegetable proliferated when it was recognized as an essential source of alpha and b- carotenes and provitamin A.[10]

Along with neuro, gastro, and hepatoprotective properties, Daucus Carota has essential anti-inflammatory effects. Porchezhian and others.[10-11] have shown the anti-inflammatory activity of the substances present in Daucus Carota. Mrohue, Nishino, and others.[11-12] have shown its anticancer activity. Yeum, Stahl, and others.[11,13] have shown its antioxidant activity. Carotenoids can scavenge oxidizing free radicals. Antioxidants are essential for the functioning of the immune system.[14]

This work presents the interactions between the amino acids of the SARS-CoV-2 coronavirus proteins and RTN and other components present, mainly in Daucus Carota. Knowledge of these interactions is essential for future product developments to prevent and treat diseases such as COVID-19.

MATERIALS AND METHOD

HyperChem is a sophisticated molecular modeling environment known for its quality, flexibility, and ease of use. By combining 3D visualization and animation with quantum chemical calculations, molecular mechanics, and dynamics, HyperChem has many molecular modeling tools to bring the researcher an extraordinary calculation power in a Windows program.[16]

The semiempirical method PM3 (Parametric Method 3) is used in hyperchem as the basis for all calculations. This method treats the molecule as a collection of valence electrons and atomic centers; each center consists of an atom and its inner electrons. The PM3 method takes molecular valence energy, including internuclear repulsion, as the sum of purely electric energy.[17]

Table 1 lists the general and specific parameters for the calculation of the HOMO and LUMO values. These parameters are calculated by trial and error until the values are approximate minimums.[18-26]

Table 1: Parameters used for quantum computing molecular orbitals HOMO 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 lists the specific parameters to calculate the electrostatic potential.

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	

RESULTS AND DISCUSSIONS

Table 3 shows the calculations of the ETCs of each of the AA and the RTN as pure substances. Column 1 shows us the order number in the quantum well. We can see that an order is descending. Columns 2 through 10 show the calculations resulting from applying the ETC theory from molecule to molecule. Column 6 (BG) shows us the forbidden band energy results, while column 9 (EP) shows us the result of the electrostatic potentials of each molecule.

Table 3: ETCs of the pure substances AA and RTN.

N	Reducing Agent	Oxidizing Agent	HOMO	LUMO	BG(eV)	δ–	δ+	EP(V/a)	ETC
21	Val	Val	-9.914	0.931	10.845	-0.131	0.109	0.240	45.188
20	Ala	Ala	-9.879	0.749	10.628	-0.124	0.132	0.256	41.515
19	Leu	Leu	-9.645	0.922	10.567	-0.126	0.130	0.256	41.279
18	Phe	Phe	-9.553	0.283	9.836	-0.126	0.127	0.253	38.879
17	Gly	Gly	-9.902	0.902	10.804	-0.137	0.159	0.296	36.500
16	Ser	Ser	-10.156	0.565	10.721	-0.108	0.198	0.306	35.037
15	Cys	Cys	-9.639	-0.236	9.403	-0.129	0.140	0.269	34.956
14	Glu	Glu	-10.374	0.438	10.812	-0.111	0.201	0.312	34.655
13	Ile	Ile	-9.872	0.972	10.844	-0.128	0.188	0.316	34.316
12	Thr	Thr	-9.896	0.832	10.728	-0.123	0.191	0.314	34.167
11	Gln	Gln	-10.023	0.755	10.778	-0.124	0.192	0.316	34.108
10	Asp	Asp	-10.370	0.420	10.790	-0.118	0.204	0.322	33.509
9	Asn	Asn	-9.929	0.644	10.573	-0.125	0.193	0.318	33.249
8	Lys	Lys	-9.521	0.943	10.463	-0.127	0.195	0.322	32.495
7	Pro	Pro	-9.447	0.792	10.238	-0.128	0.191	0.319	32.095
6	Trp	Trp	-8.299	0.133	8.431	-0.112	0.155	0.267	31.577
5	Tyr	Tyr	-9.056	0.293	9.349	-0.123	0.193	0.316	29.584
4	His	His	-9.307	0.503	9.811	-0.169	0.171	0.340	28.855
3	Met	Met	-9.062	0.145	9.207	-0.134	0.192	0.326	28.243
2	Arg	Arg	-9.176	0.558	9.734	-0.165	0.199	0.364	26.742
1	RTN	RTN	-8.218	-0.526	7.692	-0.108	0.193	0.301	25.555
Units: eV = Electron-volt, a = Bohr radius; if, a = 1, and V is for 1 e^-, then ETC is adimensional.									

On the other hand, the RTN interaction is number 1 and is located at the bottom of the quantum well. This ordination means that RTN is very stable concerning the 20 AA that makes up the proteins of sars-cov-2 and humans.

Table 4 shows the mixture "all against all" (ordination of all AA taken two by two). Thirty interactions of the first quartile are presented. The total of quantum interactions is 441. It can be noted that RTN is an excellent oxidant of the AAs of the proteins of both sars-cov-2 and the GLUT transporters, SGTL, among other proteins.

Table 4: "Quantum ordination" in the Quantum Well. 21 interactions out of 441 total.

N	Reducing Agent	Oxidizing Agent	HOMO	LUMO	BG(eV)	δ–	δ+	EP(V/a)	ETC
…22 to 441									
21	His	Asn	-9.307	0.644	9.952	-0.169	0.193	0.362	27.491
20	Arg	Asn	-9.176	0.644	9.820	-0.165	0.193	0.358	27.431
19	Tyr	RTN	-9.056	-0.526	8.530	-0.123	0.193	0.316	26.992
18	His	Ser	-9.307	0.565	9.872	-0.169	0.198	0.367	26.900

17	Arg	Ser	-9.176	0.565	9.741	-0.165	0.198	0.363	26.835
16	His	Arg	-9.307	0.558	9.865	-0.169	0.199	0.368	26.808
15	Arg	Arg	-9.176	0.558	9.734	-0.165	0.199	0.364	26.742
14	Arg	Arg	-9.176	0.558	9.734	-0.165	0.199	0.364	26.742
13	His	Tyr	-9.307	0.293	9.600	-0.169	0.193	0.362	26.519
12	Arg	Tyr	-9.176	0.293	9.469	-0.165	0.193	0.358	26.449
11	His	Glu	-9.307	0.438	9.746	-0.169	0.201	0.370	26.340
10	Arg	Glu	-9.176	0.438	9.615	-0.165	0.201	0.366	26.269
9	His	Met	-9.307	0.145	9.453	-0.169	0.192	0.361	26.184
8	Arg	Met	-9.176	0.145	9.321	-0.165	0.192	0.357	26.110
7	Met	RTN	-9.062	-0.526	8.536	-0.134	0.193	0.327	26.103
6	His	Asp	-9.307	0.420	9.728	-0.169	0.204	0.373	26.079
5	Arg	Asp	-9.176	0.420	9.596	-0.165	0.204	0.369	26.006
4	RTN	RTN	-8.218	-0.526	7.692	-0.108	0.193	0.301	25.555
3	Trp	RTN	-8.299	-0.526	7.772	-0.112	0.193	0.305	25.482
2	His	RTN	-9.307	-0.526	8.781	-0.169	0.193	0.362	24.257
1	Arg	RTN	-9.176	-0.526	8.650	-0.165	0.193	0.358	24.161

Units: eV = Electron-volt, a = Bohr radius; if, a = 1, and V is for 1 e^-, then ETC is adimensional.

Figure 1 shows the quantum well of all the interactions of the AAs of the SARS-COV2 proteins and the RTN. 18 oxidant and 12 antioxidant interactions are detailed in the first quartile. These interactions are the strongest and most likely.

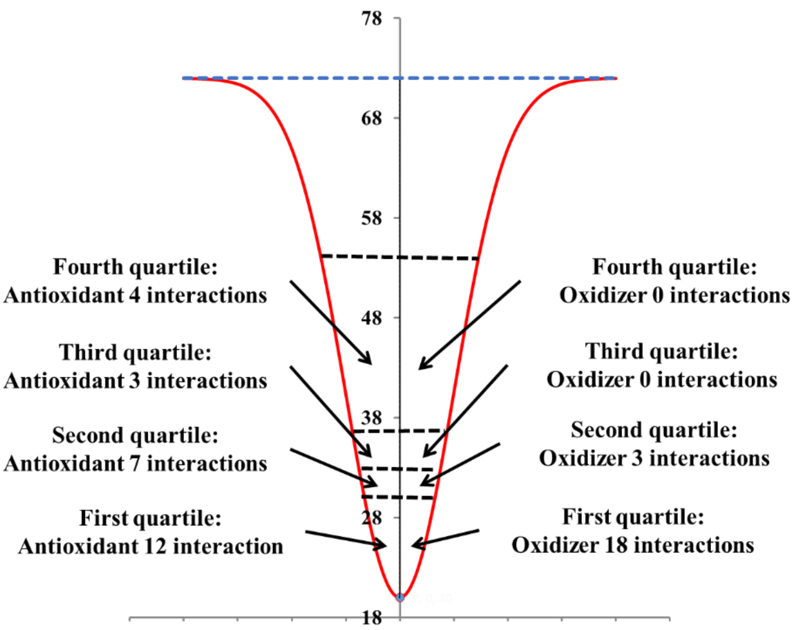

Figure 1: Quantum well of AA interactions of sars-cov-2 proteins and RTN The first quartile presents 30 interactions of the strongest and most probable.

Table 5 shows us a summary of all the quantum wells of some components of the carrot. The distributions of all interactions can be observed according to their quartile. It should be noted that with a single glass of carrot juice (200 ml), we can combat sars-cov-2 and also strengthen the immune system. This strengthening of the immune system is shown in table 6, which indicates each person's daily requirement.

Table 5: Comparison of the interactions of *RTN and, other chemical compounds in carrots.

	First quartile			Second quartile			Third quartile			Fourth quartile			
Substance	R	O	**Total**	R	O	**Total**	R	O	**Total**	R	O	**Total**	**Grand total**
*RTN	12	18	**30**	4	3	**7**	2	0	**2**	3	0	**3**	**42**
Biotin	7	18	**25**	7	3	**10**	3	0	**3**	4	0	**4**	**42**
Vitamin k	0	20	**20**	0	0	**0**	0	0	**0**	0	21	**21**	**42**
β-carotene	0	11	**11**	0	6	**6**	0	3	**3**	21	1	**22**	**42**
Total	19	67	**86**	11	12	**23**	5	3	**8**	28	22	**50**	**168**
R = Reducing agent, O = Oxidizing Agent													

Table 6: Daily requirements of some chemical constituents of carrot (WHO).

Vitamin	**% daily required per standard portion**
RTN	93
Biotina	Inaccurate[15]
Vitamin K	13
□-carotene	77

Table 7 summarizes the interactions of AA of the sars-cov-2 proteins vs. some drugs. These medications are generally prescribed one at a time for fear of interaction between them. It is observed that none of them compete in terms of efficacy and efficiency with carrots and other fruits, legumes, and vegetables.

Table 7: Comparison of the interactions of AA of sars-cov-2 and, other medicaments.

	First quartile			Second quartile			Third quartile			Fourth quartile			
Substance	R	O	**Total**	R	O	**Total**	R	O	**Total**	R	O	**Total**	**Grand total**
Favipiravir	2	21	**23**	9	0	**9**	5	0	**5**	5	0	**5**	**42**
Remdesivir	1	21	**22**	7	0	**7**	7	0	**7**	6	0	**6**	**42**
Ac. Acetilsalicílico	1	21	**22**	7	0	**7**	8	0	**8**	5	0	**5**	**42**
Ivermectina	8	11	**19**	7	7	**14**	2	3	**5**	4	0	**4**	**42**
R = Reducing agent, O = Oxidizing Agent													

CONCLUSIONS

We have calculated the chemical-quantum interactions of the AAs of the sars-cov-2 proteins vs. RTN, and we have found that.

1. RTN is the most stable substance between the 20 AA of the sars-cov-2 proteins and the AA of humans (Table 3).
2. RTN is an oxidizing agent with 18 interactions in the first quartile of the quantum well.
3. RTN is an anti-oxidant agent with 12 interactions in the first quartile of the quantum well.
4. The first quartile has 30 chemical-quantum interactions in total.
5. Carrot has other chemical compounds similar to RTN, and together they increase the power to fight sars-cov-2 (Table 5).
6. No allopathic medicine is comparable to these natural substances to fight sars-cov-2. Tables 5, 6, and 7.
7. We invite the public to strengthen their immune system with these natural substances to combat Sars-CoV-2.

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