WORLD JOURNAL OF PHARMACEUTICAL RESEARCH
SJIF Impact Factor 8.084
Volume 10, Issue 10, 23-31. Research Article ISSN 2277– 7105

ANALYSIS OF CHEMICAL-QUANTUM INTERACTIONS BETWEEN QUERCETIN, SARS-COV-2 PROTEINS, AND COVID-19

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Article Received on
08 June 2021,
Revised on 28 June 2021,
Accepted on 18 July 2021
DOI: 10.20959/wjpr202110-21125

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ABSTRACT

Flavonoids or phenolic acids are antioxidants present in plants. Quercetin (QCT) is a carbohydrate-free flavonoid, very abundant in vegetables and fruits. This compound has a wide range of antioxidant, anti-inflammatory, and immune-regulating effects and cardiac and neurological protection. The objective of this article was to analyze the chemical-quantum interactions between quercetin and the spike proteins of the sars-cov-2 causing covid-19. Hyperchem software was used to carry out all simulations. The ETC theory was used to calculate this coefficient to rank the interactions. As a result, the oxide-reduction interactions of QCT vs. AAs from sars-cov-2 proteins. Sixty-one interactions were made. The predominant oxidation interactions in quartile I am 15 and 6 in quartile II. There are no predominant reduction interactions in quartile I. There are only five predominant reduction interactions in quartile II. In total, 26 interactions can inactivate or destroy sars-cov-2 proteins. As a general conclusion, we have found that QCT can neutralize or even destroy sars-cov-2 and, at the same time, strengthen the human immune system.

KEYWORDS: Quantum chemistry, Quercetin, Proteins, Amino acids, Sars-Cov-2, Covid-19.

INTRODUCTION

Flavonoids or phenolic acids are antioxidants present in plants. QCT is a carbohydrate-free flavonoid, very abundant in vegetables and fruits. This compound has a wide range of antioxidant, anti-inflammatory, and immune-regulating effects and cardiac and neurological protection.[1]

SARS-CoV-2 is the coronavirus designation that causes the disease called COVID-19 and the pandemic 2020 - 2021. This virus is of the RNA type with 30,000 nucleotides in four genes.[2] The molecules that make up this biological material can react with compounds such as QCT. One of the vegetables with the highest QCT content is onion.[3,4]

Onion is traditionally considered a healthy plant due to its nutritional properties according to people's beliefs.[5] Onion (Allium Cepa L.) belongs to the Liliaceae family (Liliaceae) together with garlic and numerous ornamental flower plants.[6]

Historical records of onion use date back at least 5000 years. The region of origin of the onion is not demonstrated. It is probably native to the area of Asia that includes northwestern India, Baluchistan, and Afghanistan. In the oldest recorded history in the tombs of Egypt in 3200 BC, onions were eaten as food. It is believed that the Egyptians used them to feed the workers to give them the strength to build pyramids.[7,8] References to onion as a portion of food are also found in the Bible and the Koran. The Greeks and Romans also used onions. When the Romans introduced the onion to Europe, it quickly became a popular vegetable. Today, onion continues to be an essential part of many people's daily diets around the world.[5,9]

Torija and collaborators have reported evidence of the medicinal use of onion throughout the history of humankind.[10] Clare and his team have described the biological processes of onion in its use as a medicine.[9,11] Galmarini and his team have analyzed the physiological effects of various components of onions.[12,13] Derosa and his team have reported positive relationships between QCT and other components of onion as a preventive substance for COVID-19 disease.[14-17]

This work reports the quantum chemical analysis of QCT, the main component of onion, related to the nucleotides that make up the Sars-CoV-2 virus to discover potential uses of this substance to benefit health.

MATERIALS AND METHOD

Hyperchem software was used to carry out all simulations. The ETC theory was used to calculate this coefficient to rank the interactions.[18]

Below are the specific parameter tables.

Table 1 shows the general parameters of the simulator. For energy minimization, the Polak-Rebiere model was used.

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

In table 2. We use the parameter 0.015 to measure the surfaces of the molecules. In previous articles, this parameter was used to standardize the calculations.

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	

The ETC is the parameter that helps us to rank and compare all interactions.

$$ETC = \frac{|BG|}{EP}$$ Equation 1

Where:

BG = Band Bag (acronym in English)

EP = Electrostatic potential.

ETC = Electron Transfer Coefficient.

Each table is a summary of these calculations.

We obtained the calculations of each of the orbitals and electrostatic potentials of the QCT. Figure 1 shows us the molecular images of the calculations that were used in each of the tables.

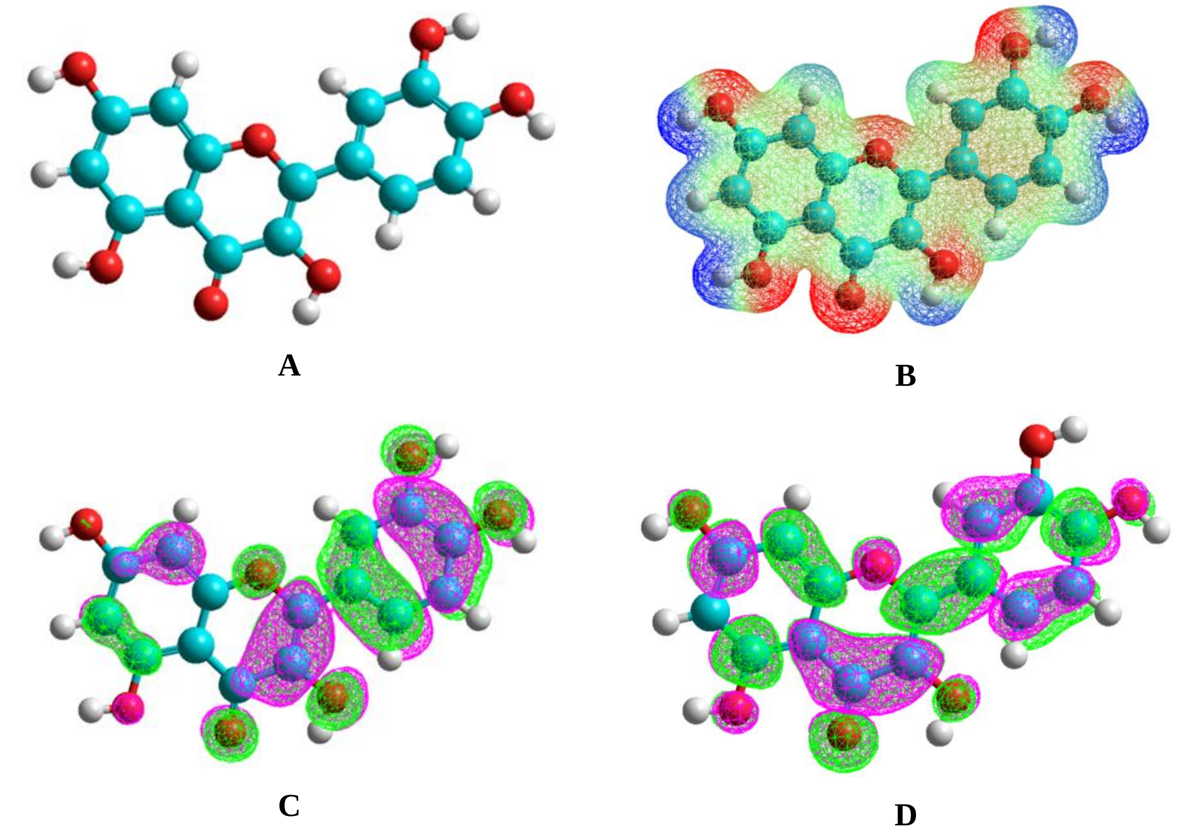

Figure 1: QCT molecule A) Cylinders and balls model. B) Electrostatic map. C) HOMO. D) LUMO.[19-21]

RESULTS AND DISCUSSIONS

The first thing that was done was the characterization of the Sars-cov-2 proteins. Table 3 lists this characterization. The statistical mode 107 units of the AA Leu is observed. This mode matches all the statistical modes of the GLUT and SGTL glucose transporters.

Table 3: Characterization of the proteins of the spikes of Sars-cov-2.

AAs	Amount	Percentaje
Ala	81	6.29%
Arg	42	3.26%
Asn	88	6.83%
Asp	61	4.74%
Cys	30	2.33%
Gln	66	5.12%
Glu	51	3.96%
Gly	94	7.30%
His	26	2.02%
Ile	71	5.51%
Leu	107	8.31%
Lys	58	4.50%
Met	11	0.85%
Phe	79	6.13%
Pro	63	4.89%
Ser	105	8.15%
Thr	95	7.38%
Trp	12	0.93%
Tyr	53	4.11%
Val	95	7.38%
	1288	100.00%

In table 4, the competing interactions of the pure amino acids concerning QCT are presented. QCT ranks second in interaction in the table. This position indicates that QCT is very stable for all amino acids except arginine. This substance is long-acting when it interacts with amino acids in proteins. The previous point justifies why the onion smell lasts so long when ingested. The attack on the sars-cov-2 proteins is also explained.

On the other hand, QCT can attack human proteins. Nevertheless, humans have metabolized QCT for millions of years; that is, we have a metabolism to process QCT correctly. Sars-cov-2 does not have as advanced a metabolism as humans. This lack of metabolism of sars-cov-2 can lead to inactivation or destruction.

Table 4: Amino Acids and Ordered substances. Quantum well. It is observed that QCT remained as interaction 2 of this well.

N	Reducing agent	Oxidizing agent	HOMO	LUMO	BG	E-	E+	EP	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	*QCT*	*QCT*	*-8.573*	*-0.752*	*7.821*	*-0.084*	*0.206*	*0.290*	*26.968*
1	Arg	Arg	-9.176	0.558	9.734	-0.165	0.199	0.364	26.742

Table 5 shows the oxide-reduction interactions of QCT vs. AAs from sars-cov-2 proteins. Sixty-one interactions were made. Interactions in quartiles III and IV were hidden for reasons of space. The predominant oxidation interactions in quartile. Its are 15 and 6 in quartile II. There are no predominant reduction interactions in quartile I. There are only five predominant reduction interactions in quartile II. In total, 26 interactions can inactivate or destroy sars-cov-2 proteins.

Tabla 5: Interacciones oxido-reducción aminoácidos vs. QCT.

N	Reducing agent	Oxidizing agent	HOMO	LUMO	BG	E-	E+	EP	ETC
61	QCT	Val	-8.573	0.931	9.504	-0.084	0.109	0.193	49.245
Hidden interactions									
32	QCT	Arg	-8.573	0.558	9.131	-0.084	0.199	0.283	32.265
31	Pro	Pro	-9.447	0.792	10.238	-0.128	0.191	0.319	32.095
30	QCT	Tyr	-8.573	0.293	8.866	-0.084	0.193	0.277	32.006
29	QCT	Glu	-8.573	0.438	9.011	-0.084	0.201	0.285	31.619
28	QCT	Met	-8.573	0.145	8.718	-0.084	0.192	0.276	31.588
27	Trp	Trp	-8.299	0.133	8.431	-0.112	0.155	0.267	31.577
26	QCT	Asp	-8.573	0.420	8.993	-0.084	0.204	0.288	31.227
25	Glu	QCT	-10.374	-0.752	9.622	-0.111	0.206	0.317	30.353
24	Ser	QCT	-10.156	-0.752	9.404	-0.108	0.206	0.314	29.949
23	Asp	QCT	-10.370	-0.752	9.618	-0.118	0.206	0.324	29.684
22	Tyr	Tyr	-9.056	0.293	9.349	-0.123	0.193	0.316	29.584
21	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
19	Gln	QCT	-10.023	-0.752	9.271	-0.124	0.206	0.330	28.093

18	Thr	QCT	-9.896	-0.752	9.144	-0.123	0.206	0.329	27.794
17	Asn	QCT	-9.929	-0.752	9.177	-0.125	0.206	0.331	27.724
16	Ala	QCT	-9.879	-0.752	9.126	-0.124	0.206	0.330	27.656
15	Ile	QCT	-9.872	-0.752	9.120	-0.128	0.206	0.334	27.305
14	Val	QCT	-9.914	-0.752	9.161	-0.131	0.206	0.337	27.185
13	QCT	QCT	-8.573	-0.752	7.821	-0.084	0.206	0.290	26.968
12	Leu	QCT	-9.645	-0.752	8.893	-0.126	0.206	0.332	26.786
11	Arg	Arg	-9.176	0.558	9.734	-0.165	0.199	0.364	26.742
10	Gly	QCT	-9.902	-0.752	9.150	-0.137	0.206	0.343	26.677
9	Cys	QCT	-9.639	-0.752	8.886	-0.129	0.206	0.335	26.527
8	Phe	QCT	-9.553	-0.752	8.801	-0.126	0.206	0.332	26.508
7	Lys	QCT	-9.521	-0.752	8.768	-0.127	0.206	0.333	26.331
6	Pro	QCT	-9.447	-0.752	8.694	-0.128	0.206	0.334	26.030
5	Tyr	QCT	-9.056	-0.752	8.304	-0.123	0.206	0.329	25.239
4	Met	QCT	-9.062	-0.752	8.310	-0.134	0.206	0.340	24.440
3	Trp	QCT	-8.299	-0.752	7.546	-0.112	0.206	0.318	23.730
2	His	QCT	-9.307	-0.752	8.555	-0.169	0.206	0.375	22.814
1	Arg	QCT	-9.176	-0.752	8.424	-0.165	0.206	0.371	22.706
							Average:		**32.296**
							First quartile:		**27.656**

A soup of compounds was made, all against all. This soup is shown in table 6. This table shows the stable and unstable interactions of each of the 400 possible interactions.

QCT interactions are listed on the left. The AA interactions of the sars-cov-2 proteins are listed. On the right side. The amounts of interactions and the percentage they represent are shown in the middle column. QCT shows 388 (97%) stable interactions as a pure substance. For this reason, QCT is a long-acting substance, while AA interactions present 388 (97%) unstable interactions. For this reason, sars-cov-2 proteins can be altered by the presence of QCT.

Table 6: Amount interactions data of QCT vs. AAs sars-cov-2.

QCT	**Data**		**AAs**
Interactions	**Amount**	**%**	**Interactions**
Stable	388	97.00%	Unstables
Unstable	12	3.00%	Stables
Total	400	100.00%	

CONCLUSIONS

We did the following:

1. We characterize the proteins of the spikes of sars-cov-2.
2. We observe that the Leu is the statistical mode of these proteins.
3. We calculate the ETCs of the AAs that make up the sars-cov-2 proteins and the QCT.

4. We locate the ETC of the QCT as interaction number 2 of all interactions in the quantum well table 4.
5. Due to this position of the QCT in the quantum reasonably, we conclude that this substance is long-acting in the human biological system.
6. On the other hand, it was observed that QCT is a powerful oxidizing agent for AAs in sars-cov-2 proteins. Table 5.
7. We found 388 out of 400 interactions stable for QCT and the same number of unstable interactions for sars-cov-2 AAs.

As a general conclusion, we have found that QCT can neutralize or even destroy sars-cov-2 and, at the same time, strengthen the human immune system.

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