WORLD JOURNAL OF PHARMACEUTICAL RESEARCH
SJIF Impact Factor 8.084
Volume 12, Issue 10, 1-9. Research Article ISSN 2277– 7105

ANALYSIS OF PASSION FRUIT (EXTRACT PROTOCATECHUIC ACID) AS AN ANTIOXIDANT OF NUCLEIC ACIDS IN THE HUMAN BODY

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Article Received on 25 April 2023,
Revised on 14 May 2023,
Accepted on 04 June 2023
DOI: 10.20959/wjpr202310-28511

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ABSTRACT

Passion fruit (Passiflora edulis f. flavicarpa) is a potential source of phytochemical compounds with anti-proliferative properties. It is established as an approximation to the biotechnological application for this species. This investigation aimed to analyze one of the passion fruit components Protocatechuic Acid (PCA), as an antioxidant of nucleic acids in the human organism. Quantum chemistry uses hyperchem software. SE-PM3 method and Polak Reviere. It was calculated the Electron Transfer coefficient (ETC) that consists of calculating the HOMO and LUMO of a molecule in question. Then get the forbidden band (Bg). This Bg is calculated as the absolute value of the HOMO-LUMO difference. The electrostatic potential is calculated by subtracting and obtaining the absolute value of the electron densities of the molecules. The obtained value of the ETC is divided between the difference of the electronic densities or electrostatic potential. It was found that PCA is a non-prolonged-acting substance; that is, it takes a very short time inside the body. We demonstrated in silico that PCA has many health benefits, as the researchers we cited in the references reported. We found and verified that PCA is a chemically related and potent antioxidant of the BNs of DNA and RNA nucleic acids.

KEYWORDS: Passion fruit, Protocatechuic acid, Antioxidant, Amino acids, Nucleic acid, Human Body.

INTRODUCTION

The incidence of colorectal cancer has increased in the world population.[1] It has been observed that food plays a fundamental role in our lives. In general, diet is associated with consuming fruits and vegetables, reducing the risk of suffering from gastrointestinal cancer, particularly colorectal cancer.

Passion Fruit

Passion fruit (Passiflora edulis f. flavicarpa) is a potential source of phytochemical compounds with anti-proliferative properties. It is established as an approximation to the biotechnological application for this species. In addition, this fruit has anticancer activity in the neoplastic cells of the human colon.[2,3]

On the other hand, when evaluating the efficacy of the ethanolic extract of the fruit of Passiflora edulis Sims on the glycemia level in normal rats, it is concluded that this extract decreases the glycemia levels in normal rats.[4] In a study by[5] Yepes et al. (2021), they obtained the phenolic composition of the ethanolic extract of Passionflower edulis seeds. Protocatechuic acid 0.1812 □g/mg.

PCA

Song et al. (2020) comprehensively summarized the pharmacology, pharmacokinetics, and toxicity of protocatechuic acid, emphasizing its pharmacological activities discovered in the last five years. They provided updated information for future preclinical and clinical investigations of protocatechuic acid. These studies indicate that protocatechuic acid (PCA) regulates oxidative stress and inflammatory responses through multiple signaling pathways. These scientists point out that the direct effects cause other neuroprotective, antitumor, anti-osteoporotic, hepatotoxic, and nephrotoxic activities.[6]

Epidemiological evidence has shown that a high dietary intake of vegetables and fruits rich in polyphenols is associated with reduced mortality from coronary disease. Furthermore, PCA has chemopreventive potential because it inhibits chemical carcinogenesis in vitro and exerts proapoptotic and antiproliferative effects in different tissues.[7]

Other experimental studies strongly support the role of protocatechuic acid in preventing neurodegenerative processes, including Alzheimer's and Parkinson's diseases, due to its favorable influence on the processes underlying cognitive and behavioral decline, namely the accumulation of β plaques. -amyloid in brain tissues, hyperphosphorylation of tau protein in neurons, excessive formation of reactive oxygen species, and neuroinflammation. There is increasing evidence that protocatechuic acid may, in the future, become an effective and safe substance that protects against neurodegenerative disorders.[8]

The pharmacological and biological activities of PCA. It is well known for its anti-inflammatory, antioxidant, antihyperglycemic, antibacterial, anticancer, antiaging, antiatrogenic, antitumor, antiasthmatic, antiulcer, antispasmodic, and neurological properties.[9] Khan (2015) Other experiments indicate that protocatechuic acid acts through the ROCK1/Sp1/PKCγ axis and therefore has promising therapeutic potential for cardiac hypertrophy treatment.[10]

Our objective in this research was to analyze passion fruit (PCA) as an antioxidant of nucleic acids in the human organism.

MATERIAL AND METHODS

Software

Quantum chemistry was used—hyperchem software. SE-PM3 method and Polak Reviere.

Electron transfer coefficient theory

It consists of calculating the HOMO and LUMO of a molecule in question. Then get the forbidden band. This BP is calculated as the absolute value of the HOMO-LUMO difference. The electrostatic potential is calculated by subtracting and obtaining the absolute value of the electron densities of the molecules.

The obtained value of the BP is divided between the difference of the electronic densities or electrostatic potential.

The ETC of the pure substances is calculated. With this calculation distributed in a quantum well, the stability of each pure substance is obtained.

Cross-band ETCs are calculated by simulating oxidation-reduction interactions.

Finally, all cross bands against all AAs are calculated, simulating proteins. With this calculation, the chemical affinity between all AAs, including theobromine, is determined.[11-15]

Quantum well reading

Figure 1 shows the hierarchy of affinity between molecules. The highest affinity is located at the bottom of the well. The lowest affinity is shown as a supernatant in the quantum well.

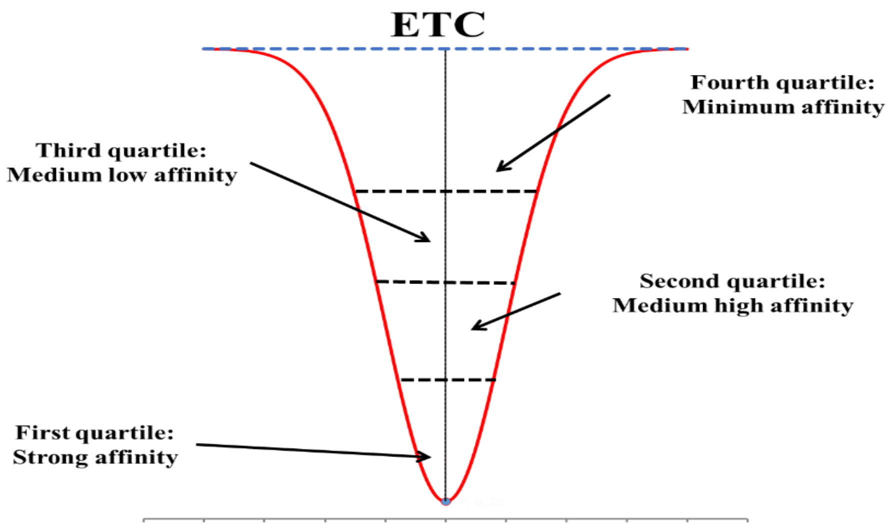

Figure 1: Quantum well reading. Substances in the first quartile are the most related and likely to occur.

RESULTS AND DISCUSSION

Figures 2 and 3 show the PCA nuclear magnetic resonance diagrams.

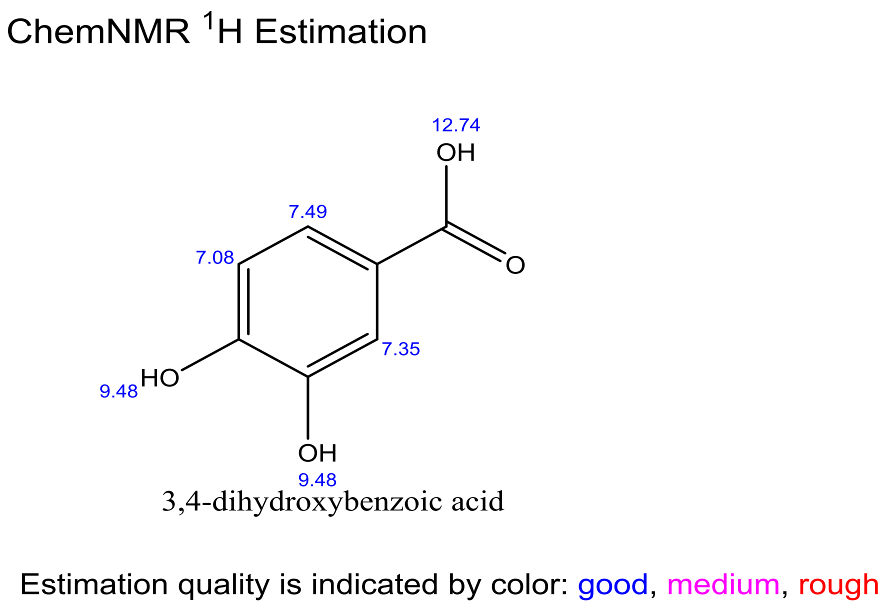

Figure 2: Location of aligned protons in NMR.

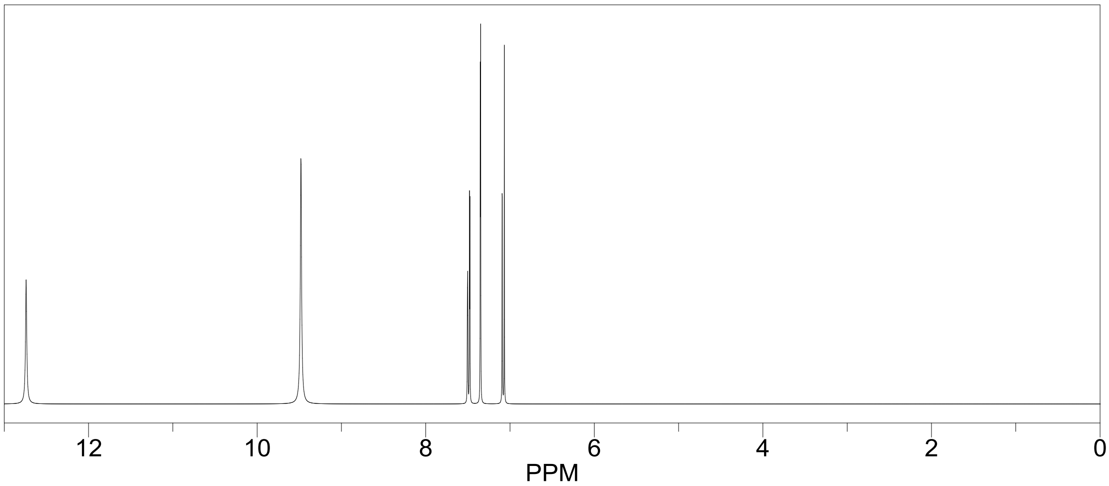

Figure 3. Diagram of NMR absorption peaks.

Table 1 shows the interactions of pure substances, including PCA. PCA is seen in 18th place. This interaction means that this acid is not long acting within the body. That is, it only remains for a while in the biological system.

Table 1: ETCs of AAS and PCA as pure substances, sorted according to the quantum well.

N	Reducing agent	Oxidizing agent	HOMO	LUMO	BG	-d	+d	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	*PCA*	*PCA*	*-7.805*	*5.613*	*13.417*	*-0.153*	*0.177*	*0.330*	*40.659*
17	Phe	Phe	-9.553	0.283	9.836	-0.126	0.127	0.253	38.879
16	Gly	Gly	-9.902	0.902	10.804	-0.137	0.159	0.296	36.500
15	Ser	Ser	-10.156	0.565	10.721	-0.108	0.198	0.306	35.037
14	Cys	Cys	-9.639	-0.236	9.403	-0.129	0.140	0.269	34.956
13	Glu	Glu	-10.374	0.438	10.812	-0.111	0.201	0.312	34.655
12	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
10	Gln	Gln	-10.023	0.755	10.778	-0.124	0.192	0.316	34.108
9	Asp	Asp	-10.370	0.420	10.790	-0.118	0.204	0.322	33.509
8	Asn	Asn	-9.929	0.644	10.573	-0.125	0.193	0.318	33.249
7	Lys	Lys	-9.521	0.943	10.463	-0.127	0.195	0.322	32.495
6	Pro	Pro	-9.447	0.792	10.238	-0.128	0.191	0.319	32.095
5	Trp	Trp	-8.299	0.133	8.431	-0.112	0.155	0.267	31.577
4	Tyr	Tyr	-9.056	0.293	9.349	-0.123	0.193	0.316	29.584
3	His	His	-9.307	0.503	9.811	-0.169	0.171	0.340	28.855
2	Met	Met	-9.062	0.145	9.207	-0.134	0.192	0.326	28.243
1	Arg	Arg	-9.176	0.558	9.734	-0.165	0.199	0.364	26.742

Table 2 shows the 21 most potent and most likely interactions of crossband PCA with AAs. PCA reduces (antioxidizes) all nitrogenous bases that will form nucleic acids. This acid generates the excellent interaction of the BNs that form nucleic acids.

Table 2: ETCs of the oxidation-reduction interactions of PCA vs. BNs.

N	Reducing agent	Oxidizing agent	HOMO	LUMO	BG	-d	+d	EP	ETC
Some interactions are omitted for reasons of space.									
19	A	T	-8.654	-0.475	8.179	-0.140	0.169	0.309	26.471
18	G	C	-8.537	-0.344	8.193	-0.150	0.161	0.311	26.345
17	C	C	-9.142	-0.344	8.798	-0.174	0.161	0.335	26.263
16	A	U1	-8.654	-0.511	8.143	-0.140	0.171	0.311	26.185
15	G	G	-8.537	-0.206	8.331	-0.150	0.172	0.322	25.873
14	C	G	-9.142	-0.206	8.936	-0.174	0.172	0.346	25.827
13	G	T	-8.537	-0.475	8.062	-0.150	0.169	0.319	25.273
12	C	T	-9.142	-0.475	8.667	-0.174	0.169	0.343	25.270
11	C	U1	-9.142	-0.511	8.631	-0.174	0.171	0.345	25.019
10	G	U1	-8.537	-0.511	8.026	-0.150	0.171	0.321	25.003
9	*PCA*	*A*	*-7.805*	*-0.213*	*7.592*	*-0.153*	*0.156*	*0.309*	*24.568*
8	A	U2	-8.654	-0.415	8.239	-0.140	0.202	0.342	24.092
7	*PCA*	*C*	*-7.805*	*-0.344*	*7.461*	*-0.153*	*0.161*	*0.314*	*23.760*
6	*PCA*	*G*	*-7.805*	*-0.206*	*7.599*	*-0.153*	*0.172*	*0.325*	*23.380*
5	C	U2	-9.142	-0.415	8.727	-0.174	0.202	0.376	23.212
4	G	U2	-8.537	-0.415	8.122	-0.150	0.202	0.352	23.074
3	*PCA*	*T*	*-7.805*	*-0.475*	*7.330*	*-0.153*	*0.169*	*0.322*	*22.763*
2	*PCA*	*U1*	*-7.805*	*-0.511*	*7.294*	*-0.153*	*0.171*	*0.324*	*22.511*
1	*PCA*	*U2*	*-7.805*	*-0.415*	*7.390*	*-0.153*	*0.202*	*0.355*	*20.816*

The box and whisker diagram presented in Figure 4 reaffirms the antioxidant view of PCA on BNs. The difference between the reducing interactions (antioxidant) left side and bottom of the diagram, and the oxidizing interactions on the right side and top of the diagram do not have an intersection. This difference means that PCA is a highly antioxidant agent of the BNs of nucleic acids.

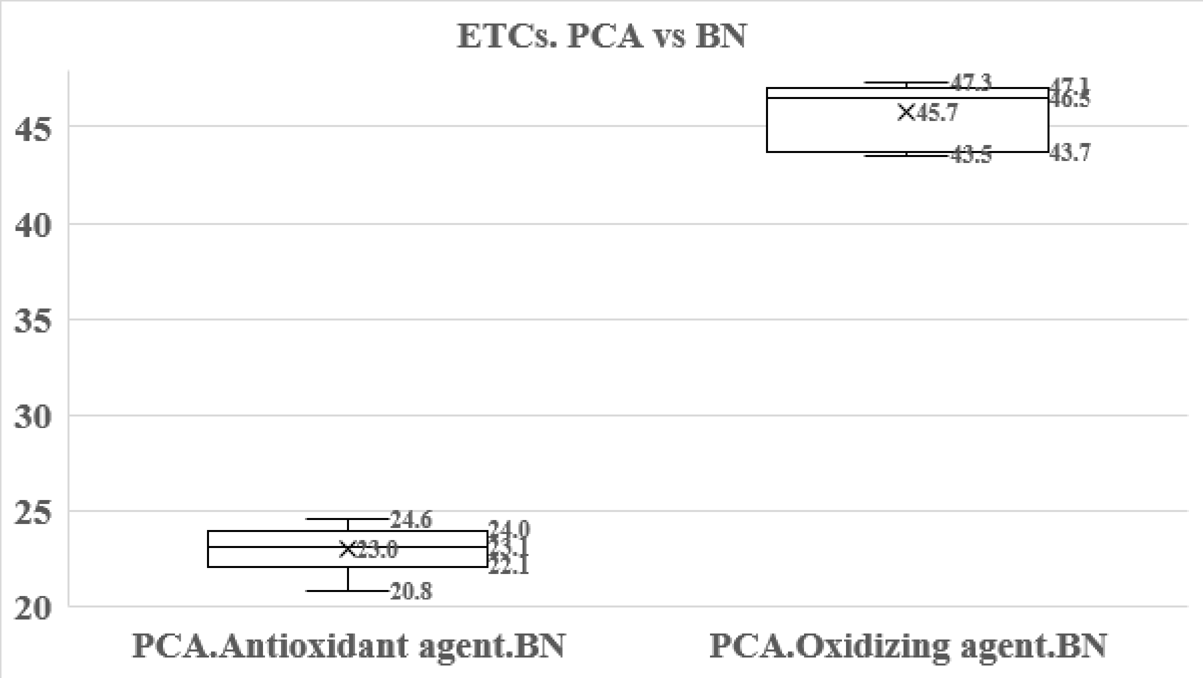

Figure 4: Box and whisker plot. Antioxidant interactions are presented on the left and below. Oxidative interactions are presented on the right side above.

CONCLUSIONES

Objective. To analyze passion fruit (PCA extract) as an antioxidant of nucleic acids in the human organism.

Hypothesis. PCA is likely to have antioxidant power on the BNs of DNA and RNA nucleic acids.

Thesis. We found and verified that PCA is a chemically related and potent antioxidant of the BNs of DNA and RNA nucleic acids—figure 4.

COROLLARIES

1. From what was previously demonstrated, it was found that PCA is a non-prolonged-acting substance; that is, it takes a very short time inside the body—table 1.
2. We demonstrated in silico that PCA has many health benefits, as the researchers we cited in the references reported.
3. Recommendations. We recommend further investigation and classification of diseases treated with PCA; We even recommend mixing PCA with other antioxidants to verify the increase or decrease of antioxidant properties.

ACKNOWLEDGMENTS

To our parents, for setting us an excellent example of honesty, persistence, and hard work to achieve desired goals.

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