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CHEMICAL-QUANTUM STUDY OF THE INTERACTIONS OF SULFORAPHANE VS. AMINO ACIDS OF THE HUMAN BEING

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ABSTRACT

Sulforaphane (SFP) is a naturally occurring isothiocyanate found in Brassica vegetables that acts as a chemopreventive agent, but its mechanism of action is unclear. This research aimed to study with quantum chemistry the interactions of sulforaphane vs. human amino acids. The Hyper Chem parameterized semi-empirical model number 3 (SE-PM3) was used to draw the corresponding molecules. We then selected SE-PM3. The geometry optimization was done with the Polak Ribiere method. It calculated the variables of HOMO-LUMO, Band gap (BG), Electrostatic Potential (EP), Electron transfer coefficient (ETC), and other properties. It is observed that the SFP interactions are very likely and related because they are at the bottom of the quantum well. SFP is an antioxidant substance for human amino acids. This thesis agrees with the theoretical and conceptual framework of this research. This SFP antioxidation was calculated with quantum chemistry, especially with the ETC theory.

Keywords: Sulforaphane, Quantum Chemistry, Cancer. Hyperchem, SE-PM3.

1. INTRODUCTION

Sulforaphane (SFP) is a naturally occurring isothiocyanate found in Brassica vegetables that acts as a chemopreventive agent, but its mechanism of action is unclear. Xie et al. (2021). This phytochemical found in cruciferous vegetables activates factor 2 related to the erythroid nuclear factor and exerts anticancer, antidiabetic, and antimicrobial effects; however, few studies have investigated its efficacy in developing alcoholism-related fibrosis. On the other hand, Ishida et al. (2021) reported that cruciferous plants, including cabbage, kale, brussels sprouts, broccoli, and wasabi, among others, have a unique role in research studies. Studies have shown that consuming these plants reduces the risk of colon, lung, breast, and prostate cancer. Janczewski (2022), in other research, and Çakır et al. (2022) evaluated the clinic of sulforaphane for weight loss and metabolic disorders associated with obesity.

Researchers such as Vanduchova et al. (2019) tell us that sulforaphane, the primary phytochemical substance in broccoli, has been shown to protect humans, reduce the risk of cardiovascular diseases, and help in autism and osteoporosis. Schepici, Bramanti, and Mazzon (2020) confirm SFP's efficacy in treating neurodegenerative diseases, including Alzheimer's (AD), Parkinson's disease, and multiple sclerosis. Finally, Russo et al. (2018) and Elkashty and Tran (2022) inform us that, in recent decades, extensive studies have reported on the possible chemopreventive activity of sulforaphane, an isothiocyanate derived from glucoraphanin, which occurs in large amounts in plants of the Brassica genus. Its effects range from protecting cells against DNA damage to the modulation of the cell cycle through pro-apoptotic, anti-angiogenesis, and anti-metastasis activities. At the molecular level, sulforaphane modulates cellular homeostasis by activating the transcription factor. With its favorable toxicological profile, SFP is a promising agent in the prevention and therapy of cancer.

This research aimed to study with quantum chemistry the interactions of sulforaphane vs. human amino acids.

2. MATERIAL AND METHODS

2.1 Hamiltonian technique.

The hamiltonian combinatorial theory performed all the valence electron jumps between each substance, atom by atom of each molecule.

2.2 Quantum methodology:

The molecular simulator Hyper Chem (HC) was purchased. (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).

We use the Hyper Chem parameterized semi-empirical model number 3 (SE-PM3) to draw the corresponding molecules. We then selected SE-PM3. He optimized the geometry with the Polak Ribiere method. He calculated the variables of HOMO-LUMO, BG, EP, and other properties. The results are displayed in column-delimited tables for each concept used in the calculations.

The specific parameters selected for each simulation were the following: SET UP. Semi-empirical method: PM3. Semiempirical Options: Load and Spin. Total Load 0. Multiplicity Turn 1. SCF Control. Convergent limit 0.01. Interaction Limit 1000. Speed Up Converge Yes. Lowest matchmaking spin. Superimposition of weighting factors Sigma-Sigma 1, Pi-Pi1. Polarizabilities were not calculated.

CALCULATION 1. Geometry optimization. Polak Ribiere algorithm (conjugate gradient). Options Termination conditions. RMS gradient of 0.1 kcal/mol or 1000 cycles maximum. Empty, yes. Screen update period one cycle.

CALCULUS 2. Orbitals. Plot orbital options Isosurface representation. Orbital contour value 0.05. Wire mesh isosurface grid. Grid meshes size Coarse. Default grid layout.

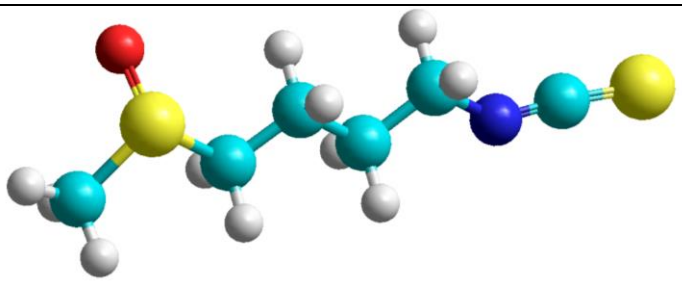
3. RESULTS AND DISCUSSION

Figure 1 presents the characterization of the sulforaphane molecule. A) Molecule in the third dimension. B) Electrostatic map; charge densities in eV/a°. C) HOMO in eV, Default beam contour. Transparency level Default.

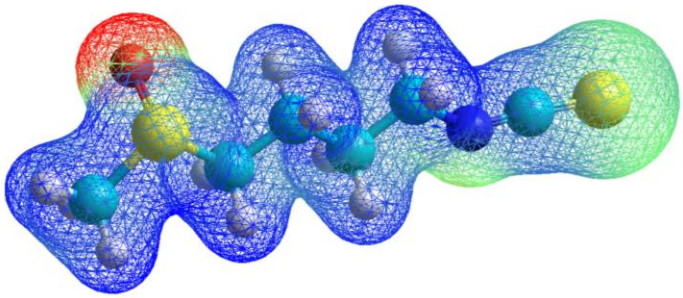
CALCULATE 3. Molecular drawings and calculations. Plot molecular options. Molecular Properties. Properties. Electrostatic potential Yes. Representations. Isosurface mapped in 3D. Grid meshes size Coarse. Default grid layout. Irregular Curve Default. A rereading of Isosurfaces. Total Charge Density Contour Value (TCDCV) 0.015. Wire mesh. Transparency level Default. We assigned options Default functions. González-Pérez et al (2017a,2017b,2022)

461 oxidation-reduction interactions of the 20 amino acids and the SFP, were made (Gonzalez-Perez *et al*. 2017). In these interactions, the antioxidants' interaction for SFP predominate.

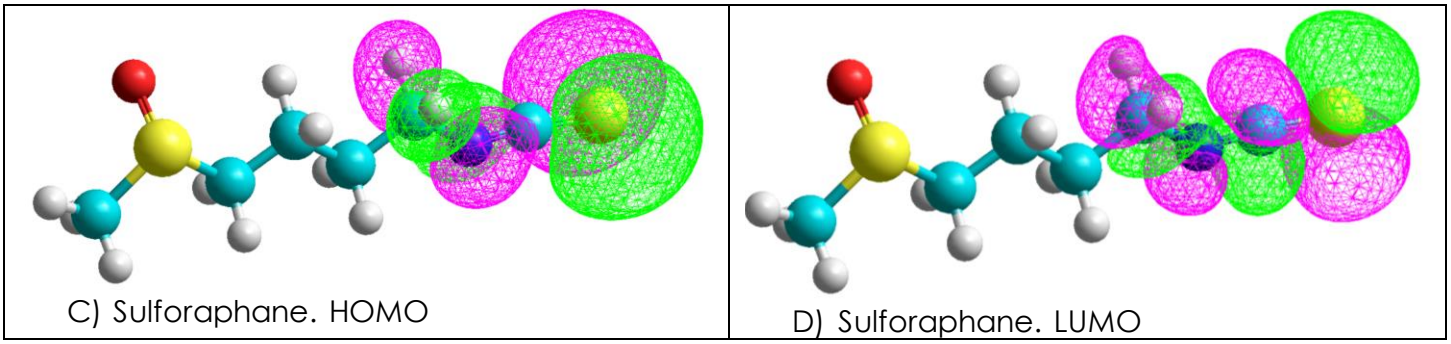
D) LUMO in eV. Where eV = electron-volts, a° = Bohr radius.
The HOMO and LUMO clouds are in a quantum superposition, which means they can form micelles when these two electron clouds overlap.



A) Sulforaphane. C = Cian, H = White, O = red, N = blue, S = Yellow.



B) Sulforaphane. Blue δ-, Red δ+, Green neutral.



C) Sulforaphane. HOMO D) Sulforaphane. LUMO

Figure 1. Sulforaphane molecule characterization using hyperchem software. A) Structure in three dimensions. B) Electrostatic map. C) HOMO, D) LUMO.

Table 1 shows the quantum calculations. The order in column 1 simulates a quantum well. Downhole interactions are more affine than pure substances. The last column represents the ETC of each substance.

Interaction number 1 (bottom of the well) is the most stable of all substances in its pure form, while interaction number 21 is the least stable and related. The interaction between SFP molecules is the most stable of all. This stability means that the SFP within the biological system is long-acting.

Table 1. Pure Amino acids and sulforaphane molecule quantum well

N	Reducing agent	Oxidizing agent	HOMO	LUMO	BG	δ-	δ+	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	Arg	Arg	-9.176	0.558	9.734	-0.165	0.199	0.364	26.742
1	SFP	SFP	-9.196	-0.761	8.435	-0.185	0.138	0.323	26.115

ETC: Electronic Transfer Coeficiente. EP?:. BG: δ-: δ+:

Table 2 shows all the possible oxidation-reduction interactions of the SFP and the 20 AAs that make up the proteins of living beings.
It is observed that the SFP interactions are very likely and related because they are at the bottom of the quantum well.
Column 1 of this table shows the number corresponding to all possible interactions, including protein sequencing. DATA numbers not listed for space reasons are natural interactions in protein sequencing.

Table 2. ETCs Oxide-Reduction Quantum well.

DATA	N	Reducing agent	Oxidizing agent	HOMO	LUMO	BG	δ-	δ+	EP	ETC
388	41	Glu	SFP	-10.374	-0.761	9.614	-0.111	0.138	0.249	38.609
379	40	Ser	SFP	-10.156	-0.761	9.396	-0.108	0.138	0.246	38.194
369	39	Asp	SFP	-10.370	-0.761	9.609	-0.118	0.138	0.256	37.536
323	38	Gln	SFP	-10.023	-0.761	9.262	-0.124	0.138	0.262	35.353
311	37	Thr	SFP	-9.896	-0.761	9.136	-0.123	0.138	0.261	35.003
305	36	Asn	SFP	-9.929	-0.761	9.168	-0.125	0.138	0.263	34.861
303	35	Ala	SFP	-9.879	-0.761	9.118	-0.124	0.138	0.262	34.802
289	34	SFP	Val	-9.196	0.931	10.127	-0.185	0.109	0.294	34.446
277	33	Ile	SFP	-9.872	-0.761	9.111	-0.128	0.138	0.266	34.254
264	32	Val	SFP	-9.914	-0.761	9.153	-0.131	0.138	0.269	34.027
246	31	Leu	SFP	-9.645	-0.761	8.885	-0.126	0.138	0.264	33.654
228	30	Phe	SFP	-9.553	-0.761	8.792	-0.126	0.138	0.264	33.304
225	29	Cys	SFP	-9.639	-0.761	8.878	-0.129	0.138	0.267	33.251
221	28	Gly	SFP	-9.902	-0.761	9.142	-0.137	0.138	0.275	33.243
218	27	Lys	SFP	-9.521	-0.761	8.760	-0.127	0.138	0.265	33.056
201	26	Pro	SFP	-9.447	-0.761	8.686	-0.128	0.138	0.266	32.654
169	25	SFP	Leu	-9.196	0.922	10.118	-0.185	0.130	0.315	32.120
152	24	Tyr	SFP	-9.056	-0.761	8.295	-0.123	0.138	0.261	31.783
134	23	SFP	Ala	-9.196	0.749	9.945	-0.185	0.132	0.317	31.372
97	22	Met	SFP	-9.062	-0.761	8.301	-0.134	0.138	0.272	30.520
91	21	SFP	Phe	-9.196	0.283	9.479	-0.185	0.127	0.312	30.382
83	20	Trp	SFP	-8.299	-0.761	7.538	-0.112	0.138	0.250	30.152
67	19	SFP	Gly	-9.196	0.902	10.097	-0.185	0.159	0.344	29.353
36	18	His	SFP	-9.307	-0.761	8.547	-0.169	0.138	0.307	27.840
33	17	Arg	SFP	-9.176	-0.761	8.416	-0.165	0.138	0.303	27.774
31	16	SFP	Cys	-9.196	-0.236	8.960	-0.185	0.140	0.325	27.570
29	15	SFP	Trp	-9.196	0.133	9.328	-0.185	0.155	0.340	27.436
27	14	SFP	Ile	-9.196	0.972	10.167	-0.185	0.188	0.373	27.259
26	13	SFP	His	-9.196	0.503	9.699	-0.185	0.171	0.356	27.244
20	12	SFP	Lys	-9.196	0.943	10.139	-0.185	0.195	0.380	26.680
19	11	SFP	Thr	-9.196	0.832	10.028	-0.185	0.191	0.376	26.670
18	10	SFP	Pro	-9.196	0.792	9.988	-0.185	0.191	0.376	26.563
15	9	SFP	Gln	-9.196	0.755	9.951	-0.185	0.192	0.377	26.394
11	8	SFP	SFP	-9.196	-0.761	8.435	-0.185	0.138	0.323	26.115
8	7	SFP	Asn	-9.196	0.644	9.840	-0.185	0.193	0.378	26.032

6	6	SFP	Ser	-9.196	0.565	9.761	-0.185	0.198	0.383	25.485
5	5	SFP	Arg	-9.196	0.558	9.754	-0.185	0.199	0.384	25.400
4	4	SFP	Tyr	-9.196	0.293	9.488	-0.185	0.193	0.378	25.101
3	3	SFP	Glu	-9.196	0.438	9.634	-0.185	0.201	0.386	24.959
2	2	SFP	Met	-9.196	0.145	9.341	-0.185	0.192	0.377	24.777
1	1	SFP	Asp	-9.196	0.420	9.616	-0.185	0.204	0.389	24.720

ETC: Electronic Transfer Coeficiente. EP:?; BG: δ-: δ+:

Figure 2 shows two whisker plots of all SFP vs. AA oxidation-reduction interactions. Reducing or antioxidant interactions are shown in the diagram on the left, and oxidizing interactions are on the right. The antioxidant interactions are more stable and chemically related by the lower values of ETCs. This location of antioxidant interactions leads us to believe that SFP is a potent antioxidant or reducing agent.

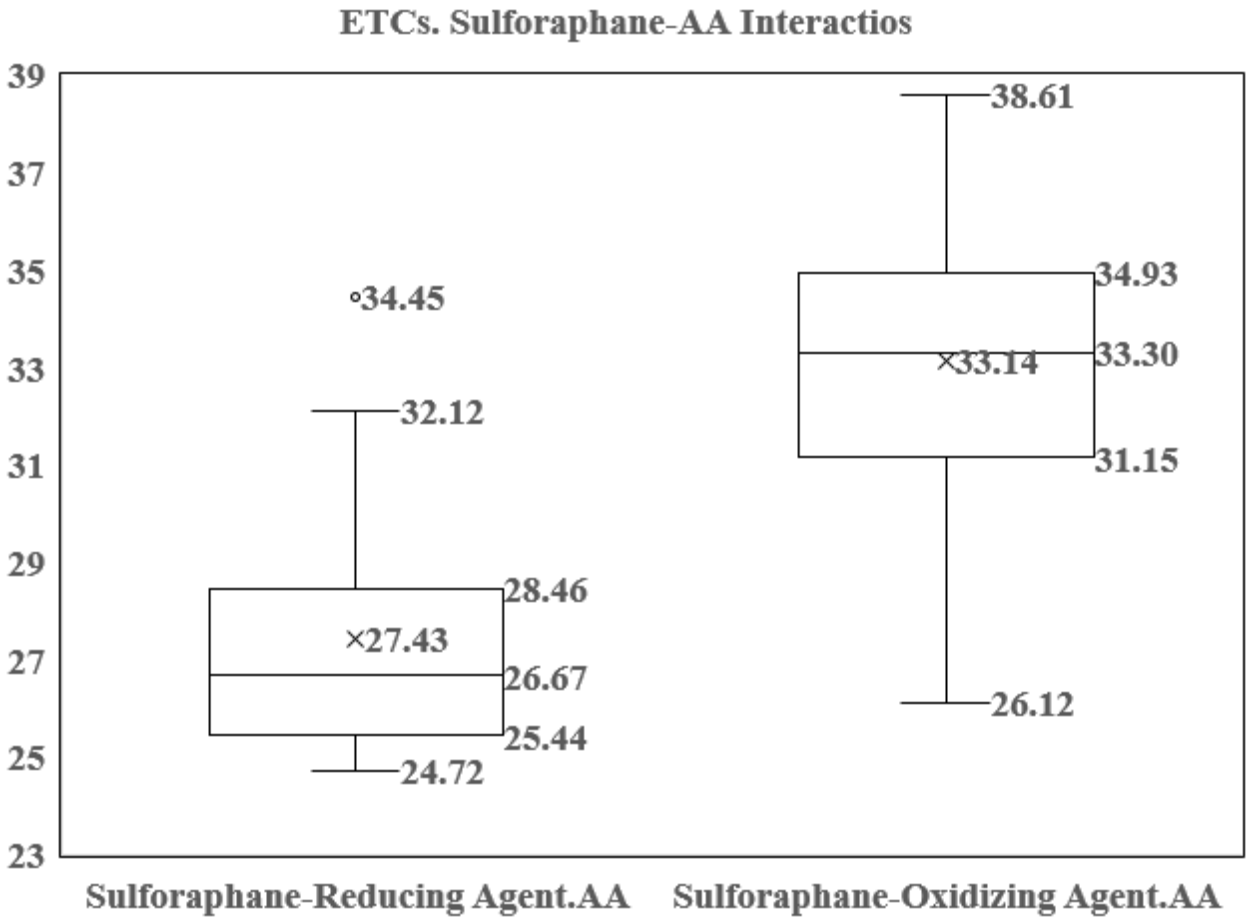


Figure 2. Oxidation-reduction diagrams. The bottom left side is antioxidant or reducing interactions. The upper right side is oxidizing interactions.

5. CONCLUSIONS

5.1 Objective. Study with quantum chemistry the interactions of SFP vs. AAs of the human being.

5.2 Thesis. SFP is an antioxidant substance for human amino acids. This thesis agrees with the theoretical and conceptual framework of this research. This SFP

antioxidation was calculated with quantum chemistry, especially with the electron transfer coefficient (ETC) theory.

5.3 Corollary and arguments. In addition to these calculations, we found at least 16 antioxidant interactions. The most probable and most potent was the SFP-Asp with an ETC = 24.720 a°.

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