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HYPOGLYCIN A: QUANTUM ANALYSIS OF THE MOLECULAR ELECTRONIC INTERACTIONS OF THE AMINO ACID PRESENT IN THE UNRIPE LYCHEE FRUIT, OVER THE ENZYMES THAT HELP IN THE PROCESS OF GLUCONEOGENESIS

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ABSTRACT

Hypoglycin A is a naturally occurring amino acid found in the unripe lychee fruit. Lychee has been linked to the Jamaican Vomiting Sickness, caused for the consumption of significant amounts of Hypoglycin A, even though some studies have found Hypo-A inhibits several enzymes in the citric acid cycle (specifically the ones that help to form acetyl-CoA). It remains unclear how Hypo-A affects the rest of the human body. The purpose of this research is using quantum semiempirical method (PM3) to determine the molecular electronic interaction of the Hypoglycin A over the enzymes that help in the process of gluconeogenesis. The content of amino acids of each enzyme is based in the National Center for Biotechnology Information (NCBI). The result of the study demonstrates Hypoglycin A has a more prominent molecular electronic interaction to valine and leucine.

Glucose-6-phosphatase, glucose-6-phosphate isomerase and triosephosphate isomerase have a significant content of valine-leucine, based in this we conclude these enzymes are more prone to suffer an effect that may cause inhibition in their functioning because to the high-value interaction of the enzymes with Hypoglycin A.

KEYWORDS: Hypoglycin-A, Semi-empirical method (SE-PM3), gluconeogenesis, lychee fruit, molecular electronic interaction, NCBI database.

INTRODUCTION

Hypoglycin or A, β-(methylenecyclopropyl) alanine is an amino acid found in a variety of fruits; more specific in the soapberry family which includes the ackee, the longan, and the lychee. Originally from Africa and then imported to Jamaica, the unripe state of the lychee fruit which will be the focus of this investigation. Lychee has been blamed for causing the called Jamaican Vomiting Sickness, linked to the consumption of a significant amount of Hypoglycin A and B, which are found in the seeds of the lychee fruit. Although, some studies have found the Hypoglycin A (Hypo-A) molecule inhibits several enzymes in the Krebs cycle; more specific the ones that help to form Acetyl-CoA. It is still unclear how the sickness works and affects the human body. Symptoms such as vomiting, convulsions and in rare cases death have induced several medical studies, biochemical and even genetic ones. It is important to stress that the Jamaican vomiting sickness (a toxic hypoglycemic syndrome) affects more people in Africa and the Caribbean than in the rest of the world.[6] NCBI (National Center for Biotechnology Information) database is a resource for molecular biology. Developed to aid in the understanding of fundamental molecular and genetic processes that control health and disease. Stored and analyzed knowledge about molecular biology, biochemistry, and genetic research was used to sustain the analysis made in this research. Information about the enzymes that help in the process of gluconeogenesis was obtained from the NCBI database and used for the computational sequencer. By using quantum semi-empirical computational methods, the molecular electronic interaction, specifically of the Hypo-A, a naturally occurring amino acid can be measured and can be compared to the enzymes that act within the gluconeogenesis. Some researchers claim that it is possible to determine the interaction between Hipo-A and the enzymes involved in glycogenesis. This determination is based on electron band theory and cross-band ETC calculations. These interactions can be studied mainly for each amino acid. According to the

amino acid content of the enzymes, it can be concluded that the gluconeogenesis process is affected or not by the inhibition of the enzymes.

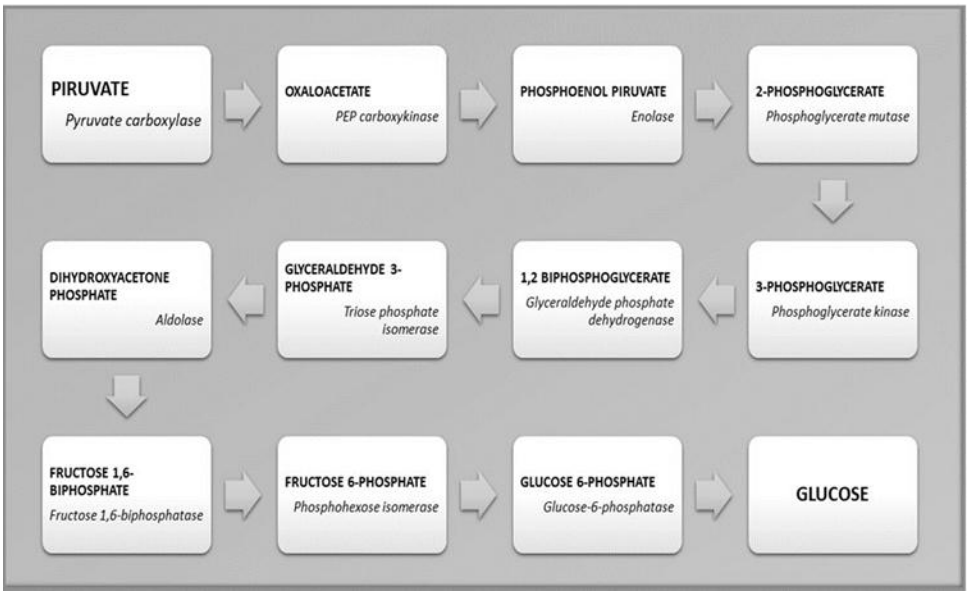

Figure 1: Gluconeogenesis process and the enzymes that take part.

MATERIAL AND METHOD

Software Hyperchem (Hypercube, Multi on for Windows, series 12-800-1501800080 Multi On, South 1236-301), was used to perform the chemical simulation of the Hypo-A molecule and the enzymes that catalyze the reactions in the gluconeogenesis process. Pyruvate carboxylase, PEP carboxykinase, enolase, phosphoglycerate mutase, phosphoglycerate kinase, glyceraldehyde phosphate dehydrogenase, triose phosphate isomerase, aldolase, fructose 1,6-biphosphatase, phosphohexose isomerase, and glucose-6-phosphatase were sequenced (Computational Sequencer) to obtain the total amino acid amount and the percentage contained by all the enzymes. The results and calculations will rely on the theory of the electron transfer coefficient.

RESULTS AND DISCUSSION

The NCBI database gave us information about every one of the enzymes involved in the gluconeogenesis process. That allowed us to use our computer sequencer that decoded the NCBI information and transformed it into data that we can see represented as the percentage of amino acids contained in each of the enzymes. The sequencing software gave us percentage values, to show which amino acid is at a more significant or smaller proportion. The molecule was built in the Hyperchem software, which was programmed to give us information about negative and positive charge values, as well as its distribution in the

molecule. In addition to its values of HOMO and LUMO. All this information was used together to perform the calculations of the ETC theory. In particular, the differences between the values of HOMO-LUMO and the values of negative potential (E-) and the positive potential (E +) must be obtained. The last calculation was to obtain a coefficient that is related to the intensity with which the Hypo-A molecule can attack by molecular oxidation to a nearby chemical species. Table 1 shows the ETC value obtained by Hyperchem Software via PM3 SE-Method for the Hypoglycin-A molecule. Also, tables 2 to 12 show the data obtained about the total composition in the percentage of amino acids based on the NCBI data for the enzymes that help in the process of gluconeogenesis.

Table1. Data obtained from hypoglycin-A USING PM3 SEMI EMPIRICAL METHOD

Reducer agent	Oxidizing agent	HOMO	LUMO	BG	E-	E+	EP	ETC
HypoA	HypoA	-9.81586	0.7186809	*10.5345419*	-0.039	2.347	*2.386*	**4.41515**

Table 2. Glucose-6-phosphatase.

Ala	20	5,60%
Arg	8	2,24%
Asn	10	2,80%
Asp	10	2,80%
Cys	7	1,96%
Gln	15	4,20%
Glu	10	2,80%
Gly	22	6,16%
His	11	3,08%
Ile	20	5,60%
Leu	51	14,29%
Lys	17	4,76%
Met	5	1,40%
Phe	25	7,00%
Pro	16	4,48%
Ser	30	8,40%
Thr	16	4,48%
Trp	13	3,64%
Tyr	16	4,48%
Val	35	9,80%
Total	357	100,00%

Table 3. Glucose-6-phosphate isomerase.

Ala	45	7,91%
Arg	30	5,27%
Asn	27	4,75%
Asp	25	4,39%
Cys	5	0,88%
Gln	31	5,45%
Glu	32	5,62%
Gly	37	6,50%
His	22	3,87%
Ile	28	4,92%
Leu	57	10,02%
Lys	35	6,15%
Met	16	2,81%
Phe	28	4,92%
Pro	27	4,75%
Ser	32	5,62%
Thr	37	6,50%
Trp	11	1,93%
Tyr	13	2,28%
Val	31	5,45%
Total	569	100,00%

Glucose-6-phosphatase

LOCUS: AAA16222 357 aa linear PRI 03-FEB-1994

DEFINITION: glucose-6-phosphatase

Glucose-6-phosphate isomerase

LOCUS: ARJ36701 559 aa linear PRI 25-APR-2017

DEFINITION: glucose-6-phosphate

[Homo sapiens].

ACCESSION: AAA16222

VERSION: AAA16222.1

DBSOURCE: accession U01120.1

KEYWORDS:

SOURCE: Homo sapiens (human)

NCBI DATA SOURCE

Table 4. Fructose-1,6-biphosphatase.

Ala	29	8,58%
Arg	13	3,85%
Asn	10	2,96%
Asp	22	6,51%
Cys	8	2,37%
Gln	9	2,66%
Glu	19	5,62%
Gly	25	7,40%
His	4	1,18%
Ile	19	5,62%
Leu	33	9,76%
Lys	25	7,40%
Met	14	4,14%
Phe	12	3,55%
Pro	16	4,73%
Ser	18	5,33%
Thr	19	5,62%
Trp	4	1,18%
Tyr	12	3,55%
Val	27	7,99%
Total	338	100,00%

Fructose-1,6-biphosphatase

LOCUS: AAC50207 338 aa linear PRI 10-JUN-2016

DEFINITION: fructose-1,6-biphosphatase [Homo sapiens].

ACCESSION: AAC50207

VERSION: AAC50207.1

DBSOURCE: accession AH006619.2

KEYWORDS:

SOURCE: Homo sapiens (human)

isomerase [Homo sapiens].

ACCESSION: ARJ36701

VERSION: ARJ36701.1

DBSOURCE: accession KY379509.1

KEYWORDS:

SOURCE: Homo sapiens (human)

NCBI DATA SOURCE

Table 5. Aldolase A.

Ala	42	11,54%
Arg	15	4,12%
Asn	15	4,12%
Asp	13	3,57%
Cys	7	1,92%
Gln	17	4,67%
Glu	24	6,59%
Gly	31	8,52%
His	9	2,47%
Ile	20	5,49%
Leu	34	9,34%
Lys	25	6,87%
Met	4	1,10%
Phe	8	2,20%
Pro	19	5,22%
Ser	21	5,77%
Thr	22	6,04%
Trp	3	0,82%
Tyr	13	3,57%
Val	22	6,04%
Total	364	100,00%

Aldolase A

LOCUS: CAA30979 364 aa linear PRI 10-FEB-1999

DEFINITION: aldolase A [Homo sapiens].

ACCESSION: CAA30979

VERSION: CAA30979.1

DBSOURCE: embl accession X12447.1

KEYWORDS:

SOURCE: Homo sapiens (human)

NCBI DATA SOURCE

NCBI DATA SOURCE

Table 6. Triosephosphate isomerase.

Ala	28	11,24%
Arg	8	3,21%
Asn	8	3,21%
Asp	12	4,82%
Cys	5	2,01%
Gln	11	4,42%
Glu	17	6,83%
Gly	25	10,04%
His	4	1,61%
Ile	15	6,02%
Leu	15	6,02%
Lys	20	8,03%
Met	3	1,20%
Phe	8	3,21%
Pro	10	4,02%
Ser	12	4,82%
Thr	14	5,62%
Trp	5	2,01%
Tyr	4	1,61%
Val	25	10,04%
Total	249	100,00%

Triosephosphate isomerase

LOCUS: CAA49379 249 aa linear PRI 14-NOV-2006

DEFINITION: triosephosphate isomerase [Homo sapiens].

ACCESSION: CAA49379

VERSION: CAA49379.1

DBSOURCE embl accession X69723.1

KEYWORDS:

SOURCE: Homo sapiens (human)

NCBI DATA SOURCE

Table 7. Glyceraldehyde-3-phosphate dehydrogenase.

Ala	31	9,25%
Arg	10	2,99%
Asn	19	5,67%
Asp	20	5,97%
Cys	3	0,90%
Gln	7	2,09%
Glu	13	3,88%
Gly	33	9,85%
His	10	2,99%
Ile	22	6,57%
Leu	19	5,67%
Lys	26	7,76%
Met	10	2,99%
Phe	14	4,18%
Pro	12	3,58%
Ser	21	6,27%
Thr	21	6,27%
Trp	3	0,90%
Tyr	9	2,69%
Val	32	9,55%
Total	335	100,00%

Glyceraldehyde-3 phosphate dehydrogenase

LOCUS: CAA25833 335 aa linear PRI 18-APR-2005

DEFINITION: glyceraldehyde-3-phosphate dehydrogenase [Homo sapiens].

ACCESSION: CAA25833

VERSION: CAA25833.1

DBSOURCE: embl accession X01677.1

KEYWORDS:

SOURCE: : Homo sapiens (human)

NCBI DATA SOURCE

Table 8. Phosphoglycerate kinase.

Ala	41	9,83%
Arg	11	2,64%
Asn	23	5,52%
Asp	23	5,52%
Cys	7	1,68%
Gln	6	1,44%
Glu	27	6,47%
Gly	40	9,59%
His	5	1,20%
Ile	19	4,56%
Leu	38	9,11%
Lys	42	10,07%
Met	14	3,36%
Phe	16	3,84%
Pro	17	4,08%
Ser	24	5,76%
Thr	17	4,08%
Trp	4	0,96%
Tyr	4	0,96%
Val	39	9,35%
Total	417	100,00%

Phosphoglycerate kinase

LOCUS: AAA60078 417 aa linear PRI 24-JAN-2017

DEFINITION: phosphoglycerate kinase [Homo sapiens].

ACCESSION: AAA60078

VERSION: AAA60078.1

DBSOURCE: accession AH002937.2

KEYWORDS:

SOURCE: Homo sapiens (human)

NCBI DATA SOURCE

Table 9. Phosphoglycerate mutase.

Ala	23	9,09%
Arg	17	6,72%
Asn	9	3,56%
Asp	10	3,95%
Cys	3	1,19%
Gln	7	2,77%
Glu	24	9,49%
Gly	18	7,11%
His	7	2,77%
Ile	15	5,93%
Leu	21	8,30%
Lys	22	8,70%
Met	9	3,56%
Phe	6	2,37%
Pro	14	5,53%
Ser	9	3,56%
Thr	14	5,53%
Trp	7	2,77%
Tyr	6	2,37%
Val	12	4,74%
Total	253	100,00%

Phosphoglycerate mutase

LOCUS: AAA64238 253 aa linear PRI 01-AUG-2016

DEFINITION: phosphoglycerate mutase [Homo sapiens].

ACCESSION: AAA64238

VERSION: AAA64238.1

DBSOURCE: accession AH003060.2

KEYWORDS:

SOURCE: Homo sapiens (human)

NCBI DATA SOURCE

Table10. Enolase

Ala	44	9,61%
Arg	19	4,15%
Asn	30	6,55%
Asp	30	6,55%
Cys	7	1,53%
Gln	10	2,18%

Table11. Phosphoenolpyruvate carboxykinase

Ala	47	7,56%
Arg	27	4,34%
Asn	29	4,66%
Asp	25	4,02%
Cys	14	2,25%
Gln	18	2,89%

Glu	28	6,11%
Gly	44	9,61%
His	7	1,53%
Ile	29	6,33%
Leu	39	8,52%
Lys	33	7,21%
Met	9	1,97%
Phe	15	3,28%
Pro	20	4,37%
Ser	25	5,46%
Thr	17	3,71%
Trp	3	0,66%
Tyr	13	2,84%
Val	36	7,86%
Total	458	100,00%

Enolase

LOCUS: CAA47179 458 aa linear PRI 18-APR-2005

DEFINITION: enolase [Homo sapiens].

ACCESSION: CAA47179

VERSION: CAA47179.1

DBSOURCE: embl accession X66610.1

KEYWORDS:

SOURCE: Homo sapiens (human)

NCBI DATA SOURCE

Glu	52	8,36%
Gly	54	8,68%
His	14	2,25%
Ile	39	6,27%
Leu	54	8,68%
Lys	39	6,27%
Met	22	3,54%
Phe	27	4,34%
Pro	43	6,91%
Ser	36	5,79%
Thr	24	3,86%
Trp	16	2,57%
Tyr	11	1,77%
Val	31	4,98%
Total	622	100,00%

Phosphoenolpyruvate carboxykinase

LOCUS: AAA02558 622 aa linear PRI 26-JUL-1993

DEFINITION: phosphoenolpyruvate carboxykinase [Homo sapiens].

ACCESSION: AAA02558

VERSION: AAA02558.1

DBSOURCE: locus HUMPHOSA accession L12760.1

KEYWORDS:

SOURCE: Homo sapiens (human)

NCBI DATA SOURCE

Table12. Pyruvate carboxylase

Ala	117	9,93%
Arg	72	6,11%
Asn	38	3,23%
Asp	61	5,18%
Cys	13	1,10%
Gln	46	3,90%
Glu	77	6,54%
Gly	94	7,98%
His	38	3,23%
Ile	56	4,75%
Leu	103	8,74%
Lys	56	4,75%
Met	35	2,97%
Phe	52	4,41%

Pro	69	5,86%
Ser	54	4,58%
Thr	59	5,01%
Trp	4	0,34%
Tyr	33	2,80%
Val	101	8,57%
Total	1178	100,00%

Pyruvate carboxylase
LOCUS: AAB31500 1178 aa linear PRI 24-JAN-1995
DEFINITION: pyruvate carboxylase [Homo sapiens].
ACCESSION: AAB31500
VERSION: AAB31500.1
DBSOURCE: accession S72370.1
KEYWORDS:
SOURCE: Homo sapiens (human)
NCBI DATA SOURCE

It was found that alanine (Ala), valine (Val), leucine (Leu) and glycine (Gly), where the most common amino acids present in the enzymes that catalyze the gluconeogenesis. Using Hyperchem software Hypo-A molecule was simulated to obtain the values of Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) to calculate the BG value (Band Gap Value), and the zones of more negative and positive charge of the molecule (E- and E+). Finally, the Electron Transfer Coefficient (ETC) was calculated.

The electron transfers coefficient value of 4.415 represents the dimensionless number of molecular electronic oxidation affinity of the Hypoglycin A molecule. In order to obtain the ETC value of the amino acids, valine (Val), alanine (ala), leucine(Leu), phenylalanine(Phe), glycine(Gly), serine(Ser), cysteine(Cys), glutamine(Glu), threonine(Thr), glutamic acid(Gln), asparagine(Asp), aspartic acid(Asn), lysine(Lys), tryptophan(Try), histidine(His), methionine(Met), arginine(Arg), Hyperchem Software was used, using the same semi-empirical method PM3/1, set at a density of 0.015. The HOMO and LUMO values are used to calculate the BG value. The E- and E+ values are used to calculate the Electrostatic Potential (EP), to posterior obtain the ETC value of the whole set of amino acids.

Table13. ETC values obtained by Hyperchem software

No.	Reducer	Oxidant	HOMO	LUMO	BG	E-	E+	EP	ETC
1	Val	Val	-9,914	0,931	10,845	-0,131	0,109	0,240	45,188
2	Ala	Ala	-9,879	0,749	10,628	-0,124	0,132	0,256	41,515
3	Leu	Leu	-9,645	0,922	10,567	-0,126	0,130	0,256	41,279
4	Phe	Phe	-9,553	0,283	9,836	-0,126	0,127	0,253	38,879
5	Gly	Gly	-9,902	0,902	10,804	-0,137	0,159	0,296	36,500
6	Ser	Ser	-10,156	0,565	10,721	-0,108	0,198	0,306	35,037
7	Cys	Cys	-9,639	-0,236	9,403	-0,129	0,140	0,269	34,956
8	Glu	Glu	-10,374	0,438	10,812	-0,111	0,201	0,312	34,655
9	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
11	Asp	Asp	-10,370	0,420	10,790	-0,118	0,204	0,322	33,509
12	Asn	Asn	-9,929	0,644	10,573	-0,125	0,193	0,318	33,249
13	Lys	Lys	-9,521	0,943	10,463	-0,127	0,195	0,322	32,495
14	Trp	Trp	-8,299	0,133	8,431	-0,112	0,155	0,267	31,577
15	Tyr	Tyr	-9,056	0,293	9,349	-0,123	0,193	0,316	29,584
16	His	His	-9,307	0,503	9,811	-0,169	0,171	0,340	28,855
17	Met	Met	-9,062	0,145	9,207	-0,134	0,192	0,326	28,243
18	Arg	Arg	-9,176	0,558	9,734	-0,165	0,199	0,364	26,742

The resulting experiment shows a tendency of Valine, Alanine, and Leucine to have the highest ETC value. If you have noticed these three amino acids are also the most abundant in the enzymes that take part in gluconeogenesis, this could correlate, though in this article should just be thought as a coincidence.

CROSS BAND CALCULATION

By taking the HOMO, LUMO, E- and E+ values of the Hypo-A and amino acids and making a cross-band calculation, which implies crossing the HOMO and LUMO values of both Hypo-A and some amino acid to get two BG values. The same way, we can cross the E- and E+ values of the amino acid and Hypo-A to obtain two different EP values, and consequently calculate two ETC values as shown in table 14.

Table 14. Data obtained in cross band calculation of Hypo-A vs amino acids. Hypo-A will be more probably oxidized by the amino acids, based in the higher ETC value.

Reducer	Oxidant	HOMO	LUMO	BG	E-	E+	EP	ETC
HypoA	Val	-9,815861	0,7186809	*10,747*	-0,039	2,347	*0,148*	**72,615186**
Val	HypoA	-9,914	0,931	*10,632*	-0,131	0,109	*2,478*	**4,291**
HypoA	Ala	-9,815861	0,7186809	*9,815861*	-0,039	2,347	*0,171*	**57,402696**
Ala	HypoA	-9,879	0,749	*10,597*	-0,124	0,132	*2,471*	**4,289**
HypoA	Leu	-9,815861	0,7186809	*10,737927*	-0,039	2,347	*0,169*	**63,538028**

Leu	HypoA	-9,645	0,922	*10,364*	-0,126	0,130	*2,473*	**4,1908516**
HypoA	Phe	-9,815861	0,7186809	*10,09917*	-0,039	2,347	*0,166*	**60,838374**
Phe	HypoA	-9,553	0,283	*10,2717*	-0,126	0,127	*2,473*	**4,1535382**
HypoA	Gly	-9,815861	0,7186809	*10,717444*	-0,039	2,347	*0,198*	**54,128503**
Gly	HypoA	-9,902	0,902	*10,621*	-0,137	0,159	*2,484*	**4,2758027**
HypoA	Ser	-9,815861	0,7186809	*10,380662*	-0,039	2,347	*0,237*	**43,800263**
Ser	HypoA	-10,156	0,565	*10,875*	-0,108	0,198	*2,455*	**4,4297763**
HypoA	Cys	-9,815861	0,7186809	*9,5803066*	-0,039	2,347	*0,179*	**53,521266**
Cys	HypoA	-9,639	-0,236	*10,357*	-0,129	0,140	*2,476*	**4,1831377**
HypoA	Glu	-9,815861	0,7186809	*10,254158*	-0,039	2,347	*0,24*	**42,725659**
Glu	HypoA	-10,374	0,438	*11,093*	-0,111	0,201	*2,458*	**4,512954**
HypoA	Thr	-9,815861	0,7186809	*10,64784*	-0,039	2,347	*0,23*	**46,294954**
Thr	HypoA	-9,896	0,832	*10,615*	-0,123	0,191	*2,470*	**4,2976202**
HypoA	Gln	-9,815861	0,7186809	*10,570736*	-0,039	2,347	*0,231*	**45,76076**
Gln	HypoA	-10,023	0,755	*10,742*	-0,124	0,192	*2,471*	**4,3471392**
HypoA	Asp	-9,815861	0,7186809	*10,235972*	-0,039	2,347	*0,243*	**42,12334**
Asp	HypoA	-10,370	0,420	*11,089*	-0,118	0,204	*2,465*	**4,4983979**
HypoA	Asn	-9,815861	0,7186809	*10,460066*	-0,039	2,347	*0,232*	**45,086491**
Asn	HypoA	-9,929	0,644	*10,648*	-0,125	0,193	*2,472*	**4,3073479**
HypoA	Lys	-9,815861	0,7186809	*10,758592*	-0,039	2,347	*0,234*	**45,97689**
Lys	HypoA	-9,521	0,943	*10,239*	-0,127	0,195	*2,474*	**4,1387574**
HypoA	Trp	-9,815861	0,7186809	*9,9484303*	-0,039	2,347	*0,194*	**51,280569**
Trp	HypoA	-8,299	0,133	*9,017*	-0,112	0,155	*2,459*	**3,6670195**
HypoA	Tyr	-9,815861	0,7186809	*10,10841*	-0,039	2,347	*0,232*	**43,570732**
Tyr	HypoA	-9,056	0,293	*9,775*	-0,123	0,193	*2,470*	**3,9573607**
HypoA	His	-9,815861	0,7186809	*10,318977*	-0,039	2,347	*0,21*	**49,137983**
His	HypoA	-9,307	0,503	*10,026*	-0,169	0,171	*2,516*	**3,9849511**
HypoA	Met	-9,815861	0,7186809	*9,9609619*	-0,039	2,347	*0,231*	**43,121047**
Met	HypoA	-9,062	0,145	*9,781*	-0,134	0,192	*2,481*	**3,9422204**
HypoA	Arg	-9,815861	0,7186809	*10,373781*	-0,039	2,347	*0,238*	**43,587313**
Arg	HypoA	-9,176	0,558	*9,895*	-0,165	0,199	*2,512*	**3,9390589**

In ETC theory the higher the value of the coefficient is, higher the probability of interaction (molecular electronic interaction). So based in the information obtained by the cross-band method we found Hypo-A will have more probability of being oxidized than reduced in comparing with amino acids. It was also found that valine will be the amino acid that interacts more efficiently with Hypo-A. Due to the higher ETC value. The following graph shows that clearly.

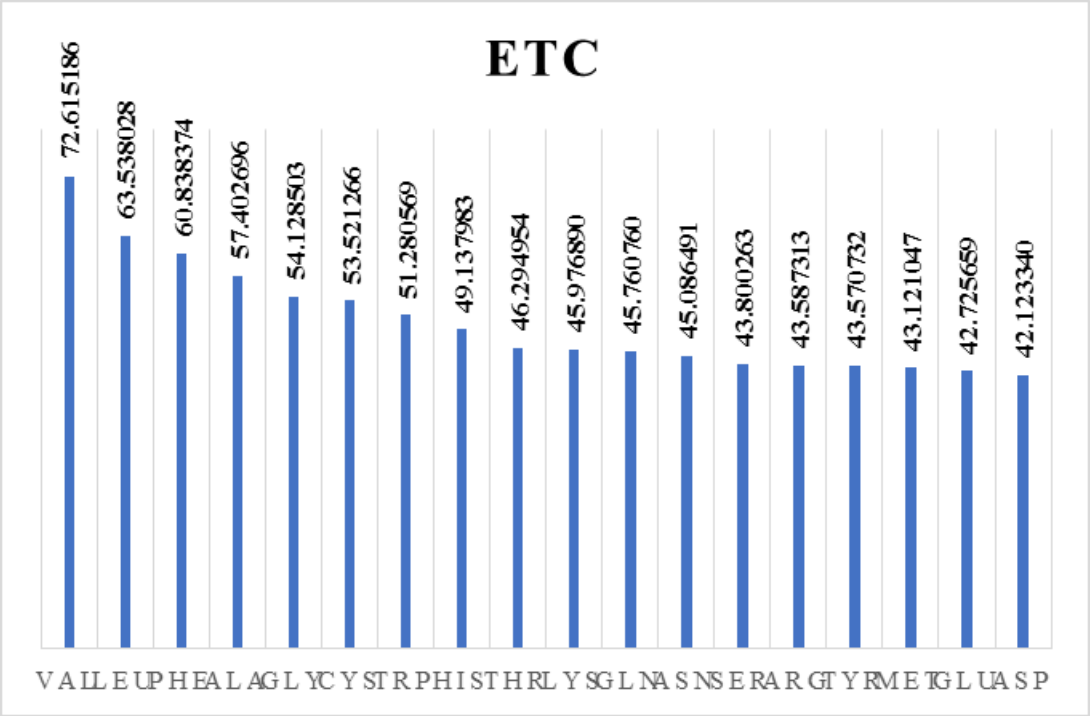

Image 2. ETC values of the HypoA-amino acid crossbanded molecules, depicting a clear tendency of valine and leucine to be the molecules with higher probability to interact with Hypo-A.

CONCLUSIONS

Based on the overall calculations, we can say that Hypoglycin-A, can have a significant molecular electronic interaction to valine and leucine. This interaction meaning that an enzyme that takes part in gluconeogenesis which has a significant proportion of leucine and valine (not considering the protein structure, and only based in electron transfers) may be affected by Hypo-A, and thus could be somehow inhibited. Under this scope glucose-6-phosphatase, glucose-6-phosphate isomerase and triosephosphate isomerase may be the enzymes that could be more effectively affected by the high ETC value of Hypo-A and thus be inhibited. The unripe lychee fruit with its high levels of Hypo-A could represent a danger cause direct affects the glucose formation, by attacking the enzymes in the last steps of the gluconeogenesis. These quantum semiempirical simulations gave us a clue about the interaction that affects the complex processes in the naturally occurring cycles such as gluconeogenesis. The use of the sequencing software and Hyperchem can complement the experimental research, and by itself can help us understand the molecular interactions in biological systems. In this article, we apply quantum semiempirical PM3 tools to measure electric potentials and electron distributions to calculate an ETC value that told us how big or small an interaction can be, between two different molecular species. The biomedical

implications can be significant because of the using of computational tools to model and measure biomolecules and their possible molecular electronic interactions within bio-systems.

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