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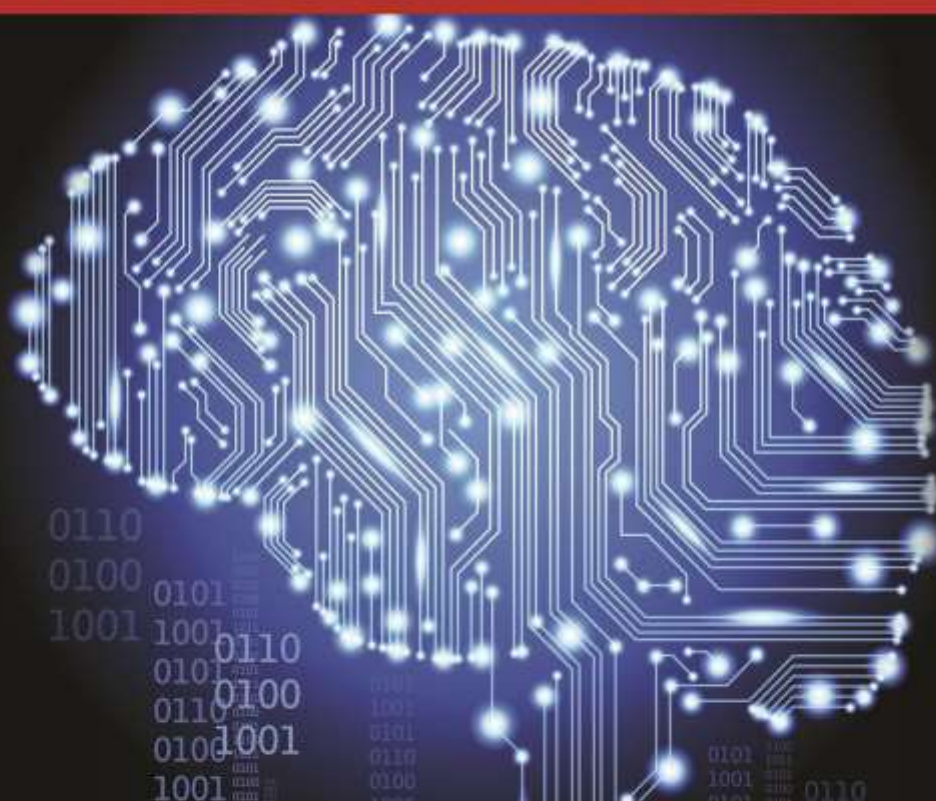
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# FOREWORD

I am pleased to put into the hands of readers Volume-4; Issue-11: Nov, 2018 of “**International Journal of Advanced Engineering, Management and Science (IJAEMS)** (ISSN: 2354-1311)”, an international journal which publishes peer reviewed quality research papers on a wide variety of topics related to Science, Technology, Management and Humanities. Looking to the keen interest shown by the authors and readers, the editorial board has decided to release print issue also, but this decision the journal issue will be available in various library also in print and online version. This will motivate authors for quick publication of their research papers. Even with these changes our objective remains the same, that is, to encourage young researchers and academicians to think innovatively and share their research findings with others for the betterment of mankind. This journal has DOI (Digital Object Identifier) also, this will improve citation of research papers.

I thank all the authors of the research papers for contributing their scholarly articles. Despite many challenges, the entire editorial board has worked tirelessly and helped me to bring out this issue of the journal well in time. They all deserve my heartfelt thanks.

Finally, I hope the readers will make good use of this valuable research material and continue to contribute their research finding for publication in this journal. Constructive comments and suggestions from our readers are welcome for further improvement of the quality and usefulness of the journal.

With warm regards.

**Dr. Uma Choudhary**

Editor-in-Chief

Date: Dec, 2018

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# Preparing Junior High School Students in Science, Technology, Engineering and Mathematics (STEM) Track Using Journal Writing in Mathematics

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**Abstract**— The authors applied a one group pretest-posttest quasi-experimental research design to one section of GVAHS with 45 students to look into the effectiveness of journal writing in mathematics performance consequently preparing the students to technical subjects in the STEM track of the K to 12 curricula. The findings of the study revealed that journals in mathematics produce better and improved scores for students in problem solving tasks. Likewise, journal writing helped the students communicate with their Math Teacher. It can improve their abilities on how to use mathematical tools, symbols and numbers, use math models, analyze, understand and solve problems preparing them for higher mathematics and other related sciences. Also, journal writing helped students to learn how to transfer ideas clearly and convey their feelings and thoughts effectively. Likewise, it enhanced different characteristics that they can use in pursuing the STEM track and in living in the globally competitive world of work.

**Keywords**— Journal Writing, Mathematics Performance, Junior High School, STEM.

## I. INTRODUCTION

One of the aims why the Philippine Government implemented the K to 12 curricula is to develop the skill competency in the global job market. The target is to improve Filipino students' mathematical, scientific and linguistic competence so that graduates will become globally competitive and are set to obtain spot in the stiff global market [1]. According to the author in [2], "all students-regardless of where they live or their socioeconomic status and cultural backgrounds-are equally deserving of educational experiences that prepare them to be globally competent." "He added that one option

is to provide students with instructional practices that consistently engage global content, multicultural perspectives and problem solving across subject areas."

In connection with this, mathematics teachers, should think of measures that will focus on attaining the goal that students should be critical thinker, international language proficient and problem solvers. As stated by the author in [3], "writing is seen as one way to encourage critical and in-depth thinking, reflection and evaluation of understanding students." "This is one activity that can be a mechanism for assessing the level of mathematical understanding in students."

Math journaling is one of the ways to introduce writing into the Math class. When children wrote journals, they examined, expressed, and kept track of their reasoning, which was especially useful when ideas became too complex. By reading their journals, teachers could evaluate the students' progress and recognized their strengths and learning needs [4]. The writing activities were able to motivate the learner, identifying what is to be learned, and providing active involvement. With the use of writing activities, students were also able to compare, classify, analyze errors, or construct support that they encounter in the course of problem solving. The writing activities included conceptual understanding, procedural knowledge and logical thinking is a means for transforming concepts and skills. Writing engaged all students actively express and explains meaning at their own abilities [3].

This is the objective of this study. Using one-group pretest-posttest quasi-experimental research design, the researchers aimed to look into the effects of journal writing in the mathematics performance of Grade 9 students. Findings of this study can help the researchers to understand better how language and mathematics are



related and how these variables improved and aid the problem-solving competencies of students who are planning to enroll in science, technology, engineering and mathematics (STEM) track which is considered as one of the tracks in senior high school that trains the learners be globally competitive. Specifically, this study sought to find out the performance of the students in their pretest and posttest examinations, the significant difference that exists between the two tests and the contributions of journal writing in studying Mathematics 9 as experienced by the students.

## II. MATERIALS AND METHODS

This study utilized the one-group pretest-posttest quasi-experimental research design. "One of the most frequently used quasi-experimental research designs in which a single group of research participants or subjects is pretested, given some treatment or independent variable manipulation, then post tested. If the pretest and posttest scores differ significantly, then the difference may be attributed to the independent variable [5]."

The experiment was conducted at the Math Classroom PPP Building of Gabaldon Vocational Agriculture High School (GVAHS) located at Barangay Pantoc, Gabaldon, Nueva Ecija, Philippines. The classroom was clean, well-ventilated, and had enough chairs and tables. The respondents of this study were 45 students in one section of Grade 9. Informed consent from

parents and assent from the respondents were secured by the researchers before doing the experimental process for ethical considerations.

The research instruments used were the pretest and posttest questionnaires. The pre-test was given to respondents before the conduct of the study. After the pretest, the participants were exposed to treatment, which was the use of journal writing. The posttest (parallel to pretest) was given to the participants after taking up all the topics included in the study to assess the acquired learning.

The 50 problem solving items of the tests came from the test-bank of the Department of Education, Division of Nueva Ecija. The test items were item analyzed by the test experts using the item analysis template. The test was designed to measure the performance of the students on radicals and variations.

The statistical tools utilized to in this study were frequency, percentage, weighted mean and t-test. The experimental procedure lasted for 9 weeks.

## III. RESULTS AND DISCUSSIONS

### 1. Pretest Performance of the Respondents

Before the experiment was conducted, the 45 student respondents were given a pretest in Mathematics 9 about radicals and variations. The results were computed using frequency and percentage.

Table.1: Performance of the Respondents in the Pretest

Score	Verbal Description	Frequency	Percent
0 to 9	Beginning (Did not Meet Expectations)	0	0.0
10 to 19	Developing (Fairly Satisfactory)	41	91.1
20 to 29	Approaching Proficiency (Satisfactory)	4	8.9
30 to 39	Proficient (Very Satisfactory)	0	0.0
40 to 50	Advanced (Outstanding)	0	0.0
<b>Total</b>		<b>45</b>	<b>100.0</b>

Table 1 shows the performance of the respondents in their pretest. Forty-one (91.1%) got scores ranging from 10-19 with a verbal description of Developing or Fairly Satisfactory. There were 4 (8.9%) who got scores ranging from 20-29 with a verbal description of Approaching Proficiency or Satisfactory. Nobody from the respondents reached the proficient and advance level indicating that majority of the them performed low in Mathematics 9. This result is related to the findings in [6], that Filipino students' performance in mathematics is weak.

### 2. Posttest Performance of the Respondents

Table 2 shows the performance of the experimental group in their posttest. There were 14 (31.1%) respondents who earned scores ranging from 40-50 with a verbal description of Advanced or Outstanding. Thirty (66.7%) got scores ranging from 30-39 having a verbal description of Proficient or Very Satisfactory. Only one student was under Approaching Proficient or Satisfactory whose score ranged from 20-29. This shows that the respondents performed well in their posttest after they were taught using journal writing in mathematics.



Table.2: Performance of the Respondents in the Posttest

Score	Verbal Description	Frequency	Percent
0 to 9	Beginning (Did not Meet Expectations)	0	0.0
10 to 19	Developing (Fairly Satisfactory)	0	0.0
20 to 29	Approaching Proficiency (Satisfactory)	1	2.2
30 to 39	Proficient (Very Satisfactory)	30	66.7
40 to 50	Advanced (Outstanding)	14	31.1
<b>Total</b>		<b>45</b>	<b>100.0</b>

The finding of the study is similar to that of [7] who conducted a study on 7th and 8th grade math students, that despite students performed low they were more engaged in journal writing in Mathematics and thus improved their performance. This finding, along with the findings of authors in [8], might be combined to suggest that journal-writing about real-world problems would make students be engaged in class since the students see the relevance of solving Mathematics problems to their lives.

### 3. Difference between the Pretest and Posttest Performance of the Respondents.

Table 3 shows the comparison of the pretest and posttest performances of the respondents. The mean pre-test score is 16.0222 with the variance of 11.2495 while the mean post-test score is 37.0889 with the variance of 20.4465. The computed t-stat is 25.08\*\* which means that post-test result is significantly higher than the pre-test implying that journal writing in mathematics is an effective strategy in increasing the problem-solving skills and mathematics' performance of the respondents.

Table.3: Comparison of the Pretest and Posttest Results

Mathematics 9	Post-test	Pre-test
Mean	37.0889	16.0222
Variance	20.4465	11.2495
N	45	45
t Stat	25.08**	

\*\*difference is significant @ 0.01 level

This finding revealed that respondents were benefited in using journal writing in their math class. The result also shows the effectiveness of the journal writing in the mathematics performance of the students.

When the respondents were asked about what they can say about the benefits of journal writing in mathematics their top 5 are:

*"1.it helped me communicate with my Math Teacher; 2.it helped improve my ability to make and analyze problems; 3.it influenced my performance in mathematics; 4. it helped me understand how to use math to model problems; and 5.it helped me better understand problems preparing me for higher mathematics and other related sciences".*

The author in [9] mentioned that journal writings have other benefits that people may need to compete globally. He also claimed the benefits such as reducing stress and anxiety, increasing self-awareness, sharpening mental skills, genuine psychological insight, creative inspiration and motivation, strengthening ability to cope during difficult times, and overall physical and emotional well-being.

Aside from the importance of journal writing to students, the author in [10] abbreviated the importance of using journal writing in mathematics teachers. He wrote: "writing in mathematics gives me a window into my students' thoughts that I don't normally get when they just compute problems. It shows me their roadblocks, and it also gives me, as a teacher, a road map."

## IV. CONCLUSIONS AND RECOMMENDATIONS

Using journals in mathematics results to better and improved scores for students in problem solving tasks. Likewise, journal writing helped the students communicate with their Math Teacher. It can enhance

their abilities on how to utilize mathematical tools, symbols and numbers, use math models, analyze, understand and solve problems. Also, journal writing aided students to learn how to interconnect notions clearly and express their feelings and thoughts and develop different characteristics that they can use in the STEM track and subsequently in the globally competitive world of work.

As recommendations, to develop students' problem-solving skills, mathematics teachers may use journal writing in their class and provide numerous journal prompts to motivate students to enjoy journal writing. Seminars, workshops, and training on journal writing may be conducted so that Math teacher will be oriented properly with its use and nature. Likewise, administrators may support and provide avenues for teachers' advancement.

However, since this study utilized only one group pre-test-post-test design, the researchers recommend conducting a similar study using two-group control design or the Solomon four-group design to deepen the understanding of the effect of the journal writing in the problem-solving abilities and critical thinking skills of the learners. Likewise, other researchers may venture on looking into the effectiveness of journal writing in the problem-solving abilities and mathematical skills of future elementary mathematics teachers.

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# Product, pricing and promotional strategies of Restaurants in Nueva Ecija: An Assessment

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**Abstract**— Marketing plays a very important role in the organization's success; it is a must to every organization to consider strategizing their different marketing practices. The study presented the marketing strategies of restaurants in Nueva Ecija. The study aimed to assess different marketing strategies which focused on product offering, pricing and promotion of the restaurants in the province. The descriptive method of research was utilized and questionnaire served as the instrument for collecting data. Owners/ managers of eight selected restaurants in Nueva Ecija were taken as respondents. As to product/service offerings, restaurants management offered variety of food and beverages to attract customers. They also maintained the cleanliness of their places and their surroundings. They based their prices on their production cost and current market demand. Meanwhile, advertising and sales promotion were the main promotional tool used by the restaurants management. On the other hand, the restaurants management should continuously provide new variety of high quality food offerings coupled with courteous and prompt services sold at a reasonable price.

**Keywords**— marketing; pricing; product; promotion; restaurants.

## I. INTRODUCTION

Filipinos love to eat, and entrepreneurs know it. If you ask would-be-entrepreneurs about their opinion of the best business to start, a lot of them will answer — it should be food-related business. Indeed, food service business is one of the most competitive fields when it comes to business, specifically in income generation, growth and expansion.

In Nueva Ecija, restaurant business becomes an industry to watch out for as increasing number of this business is very evident mostly in the heart of the city. However, the increasing number of restaurants in the city manifests that competition gets stiffer. With this, only those businesses that geared with best practices and properly managed survive.

The extreme business competition and rapid changes in business environment have enticed many

businesses into adopting businesses practices that are said to be of great help for them to achieve excellence status. These business practices are said to be the ways that have contributed to increasing the performance such as profitability and market share of the organization. Many of the owners of the businesses that have empowered their marketing practices are still in the running for the longest time and recognized as strongest contenders in the industry.

According to Marrs (2015), the competition among restaurants is fierce, and owners need to give their all to be successful. In order for a restaurant firm to stay on the industry owners should have some new fresh ideas. Restaurant owners must be vigilant on their marketing practices so that they will be able to survive competition.

In this study, the marketing strategies of restaurant businesses in Nueva Ecija in accordance with their products, pricing and promotion were described. This study will benefit the business owners as this study provided them information on their marketing practices for them to have benchmark. It is imperative therefore, for businesses to determine their best practices and continuously nurture these to keep their good standing. Moreover, this study will serve as a roadmap to the future entrepreneurs whose idea is to putting up a food business and giving them a clearer perspective on running this type of business, perhaps a slice of secrets in achieving business excellence.

## II. METHODOLOGY

The research design utilized by the researchers in this study was the descriptive method. Questionnaire was used as the technique in gathering the data and additional interview questions prompted to the interest of the researchers. Questionnaire was structured based on the study of Sangkaworn, C. and Mujtaba, B., (n.d.). The respondents of the study were the owners of the eight selected restaurants in Nueva Ecija.

## III. RESULTS AND DISCUSSIONS

### 1. Profile of the Restaurants

Table.1: Profile of the Restaurants

Description	f	%
<i>Type of ownership</i>		
Sole proprietorship	3	37.5
Partnership	3	37.5
Corporation	2	25
TOTAL		100
<i>Number of employees</i>		
4 – 6	0	0
7 – 9	0	0
10 and above	8	100
TOTAL		100
<i>Years of Existence</i>		
2 to 5 years	5	62.5
6 to 8 years	1	12.5
9 to 11 years	1	12.5
12 to 14 years	0	0
15 years and above	1	12.5
TOTAL		100

Table 1 presents the profile of the restaurants. As to type of ownership, the table shows that three (3) restaurants were under sole proprietorship type, three (3) partnership and two (2) corporation. According to the owners, sole proprietorship is a type of business organization that is easier to manage. Partnership on the other hand, is preferred by some owners because of bigger resources that can be contributed among partners.

As to number of employees the eight restaurants have more than 10 employees. As business operation grows, restaurants employed more than 10 employees to cater growing number of customers coming to their place.

In addition, five (5) restaurants are operating for 2-5 years, one (1) is in business for 6-8 years the other one (1) is operating for 9-11 years and one (1) is in restaurant industry for more than 15 years now. Restaurant industry is fast-growing industry in Nueva Ecija as number of restaurants is increasing. According to the respondents, they really worked on their marketing strategies to survive the stiff competition and for them to stay longer in the said industry.

## 2. Marketing Strategies of Restaurants

### 2.1 Product Offering

Items 1, 4 and 6 got a weighed mean of 5.00 and rated “always”. They considered the availability of variety of food and beverages, sanitation and cleanliness of the restaurant and their surroundings and prompt courteous service.

Table.2: Marketing Strategies of Restaurants in terms of Product Offering

Product/service practices	Weighted mean	Description	Rank
1. Availability of variety of food and beverages.	5	Always	2
2. Completeness of dining facilities	4.75	Always	6.5
3. Availability of parking space	4.75	Always	6.5
4. Sanitation and cleanliness of the restaurant and their surroundings	5	Always	2
5. Good and proper ventilation	4.88	Always	4.5
6. Prompt courteous service	5	Always	2
7. Attractiveness of arrangement of the place	4.88	Always	4.5

According to the respondents, they made it sure that all the foods/beverages in the menu are available so that customers will not be disappointed. In addition, they maintained a standard of cleanliness in all corners of restaurants. Furthermore, they have trained employees to be customer-friendly, accommodating and very welcoming. The restaurant owners also provided good and proper ventilation and made their place attractive.

These were the main factors that they considered in the operation of the business in order to attract and retain loyal customers.

### 2.1 Pricing

Table.3: Marketing Strategies of Restaurants in terms of Pricing

Pricing practices	Weighted mean	Description	Rank
1. Based on cost/expense of product	4.63	Always	1
2. Based on demand	4.25	Always	3
3. Discount	4.38	Always	2
4. Based on the price of competitors	3.75	Very Often	4

As to pricing, item 1 got a weighted mean of 4.63. This means that cost/expense of the product was the primary basis in their pricing. Considerations number 2 weighted mean of 4.25 and rated “always”. According to the respondents, they sometimes adjusted their prices based on the season/demand (e.i. Valentine’s Day and Christmas). Item 3 got a weighted mean of 4.38 and rated “always”. This means that they also offered discounts to their clients. Meanwhile, item 4 got a weighted mean of 3.75 and rated “very often”. This denotes that they very often used the price of the competitors as their basis.

Since price is the only element among the P’s of marketing mix that generates income, owners of the restaurants always see to it that prices are fair and affordable in order to retain customers.

### 2.3 Promotion

Table.4: Marketing Strategies of Restaurants in terms of Promotion

Promotion	Weighted mean	Description	Rank
1. Giving customer a discount	4.38	Always	5
2. Providing additional amenities such WiFi, radio and television plus cable TV, Telephone/intercom	4.88	Always	3
3. Greeting customers and being friendly	5	Always	1.5
4. Providing customers with clean and ventilated space	5	Always	1.5
5. Giving souvenirs and gifts	3.25	Often	6

As to promotion, considerations 4 and 5 both got a weighted mean of 5.00 and rated “always”. According to the respondents, they always provided customers with clean and ventilated spaces and they greeted customers and be friendly to them. On the other hand, item 1, and 2 got a weighted mean of 4.38 and 4.88, respectively and rated “always”. This implies that they gave discount to their customers and provided additional amenities such wifi, radio and television plus cable TV, telephone/intercom.

Primarily, sales promotion is one of the promotional tools used by the owners. The above sales

promotion activities are the most common factors they considered in order to capture and maintain customers’ loyalty, considering that customers are the ones who give income to the business.

Table.5: Ways of Advertising Restaurants

Ways of advertising restaurants	Weighted Mean	Description	Rank
1. Local radio	1.88	Sometimes	4
2. Local newspaper	3.13	Often	3
3. Brochures distributed	3.38	Often	1
4. Billboard nearby	3.25	Often	2

In terms of advertisement, owners often advertised their restaurants through brochures. According to them, budget was the main consideration in their advertising campaigns. Thus, they used the cheapest means of advertising such as brochures and billboards and through local newspapers and local radio stations.

### 3. Implication of the study to Business Administration

This study was conducted to find out the marketing strategies of selected restaurants of Nueva Ecija in terms of business-related factors which covered the type of ownership, number of employees, years of existence, the level of implementation of marketing strategies in terms of product offering, pricing and promotion. Since marketing now plays a very important role in the organization’s success, it is a must to every organization to consider strategizing their different marketing practices. Presented herewith were the different considerations to which, if taken much attention would contribute to the success of company’s marketing programs.

Attention on the product, pricing and promotion aspects of the business would lead you to having a higher impact on the industry you are into. In addition, since business is about earning money, giving special attention on marketing could give an organization a favourable profit.

### IV. CONCLUSIONS AND RECOMMENDATIONS

Based on the results of the study, majority of the restaurants were under sole proprietorship and partnership, with more than 10 employees and have operated for 2-5 years now. As to product/service offering, restaurant owners considered the availability of variety of food and beverages, sanitation and cleanliness of the restaurant and their surroundings and prompt courteous service. As to pricing, cost/expense of the product was the primary basis in setting prices of

products. Whereas, advertising and sales promotion were the top promotion tools used by the restaurant owners.

Thus, restaurants' management have to improve customer satisfaction levels by providing a wide variety of products with high quality coupled with courteous and prompt services sold at a reasonable price. The restaurant owners should use other promotional techniques like social media in order to make the product more popular in the minds of existing and prospective customers. Furthermore, another study prior to the evaluation as to the effectiveness of marketing strategies of restaurants should be conducted.

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# Chemical-quantum determination of the interaction type of leflunomide and collagen and its influence on arthritis

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**Abstract**— In recent years, researchers have evaluated the clinical efficacy and safety of Leflunomide (LEF) and other medications for the treatment of rheumatoid arthritis (RA). The objective of this work was chemical-quantum calculus and determination of the interaction type of LEF and collagen and its influence on arthritis. We obtained the information about the collagen of The National Center for Biotechnology Information (NCBI). It was obtained the formula of the LEF on the page of PubChem. The quantum calculations we carry out with the hyperchem software. These calculations were made in other articles already published by us. We concluded that 13 interactions of 40 calculated are significant. These 13 interactions show that only two of them are oxidant and the other 11 are reductive.

**Keywords**— Quantum chemistry, Leflunomide, Collagen, Arthritis, Amino Acid.

## I. INTRODUCTION

In recent years, researchers have evaluated the clinical efficacy and safety of LEF (figure 1) and other medications for the treatment of rheumatoid arthritis (RA). In their results, they announced that, in the treatment of RA with these combinations, it presented the characteristics of remarkably lowering the levels of laboratory indices. [1-3] In other studies, it was concluded that a weekly dose of 50 mg of LEF showed similar benefits to the 10 mg daily dose of the same medication in the treatment of moderate to moderate rheumatoid arthritis. [4] We also compared the short-term efficacy of

LEF and Methotrexate in the treatment of RA and did not find significant statistical differences. [5] They evaluated the clinical efficacy and safety of LEF as a new immunosuppressive medicine in lupus nephritis through a meta-analysis. LEF is a promising therapy for the treatment of lupus nephritis, mainly because of the efficacy and favorable safety profile determined by a meta-analysis. [6]

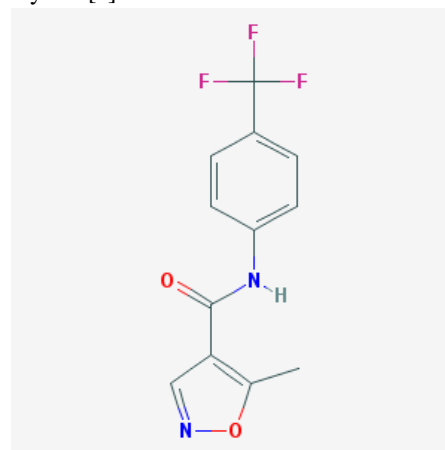


Fig.1: Leflunomide. IUPAC Name: 5-methyl-N-[4-(trifluoromethyl)phenyl]-1,2-oxazole-4-carboxamide

A proportion of patients who achieved significant clinical benefit after an adequate trial of LEF was evaluated. A significant proportion of patients, most of whom had previously failed treatment with methotrexate, were able to respond to the disease with LEF with a low risk of adverse effects, suggesting that treatment with LEF may be a reasonable and cost-effective strategy in the face of



biological therapy. [7] It was also shown that LEF could reduce the signs and symptoms of rheumatoid arthritis (RA) with regression in structural damage. Lung involvement is one of the extra-joint manifestations of rheumatoid arthritis and can occur due to any disease itself, or with medications used in the treatment. They presented 4 cases with rheumatoid arthritis that developed pulmonary nodules with LEF therapy. [8] On the other hand, a retrospective study was carried out evaluating the side effects of LE Fin 40 patients. LEF therapy was maintained in all patients and hypoglycemia regressed at variable intervals of no more than six months. They

investigated that the active metabolite of LEF A77 1726, was able to block pre-established cardiac hypertrophy in mice. Other researchers, investigated the protective effects of LEF as a new immunosuppressant, on interstitial tubule lesions in a model of diabetic nephropathy in rats. These findings suggest that LEF protects the renal lesion of diabetic rats and that it could through the inhibition of OPN / TGF- $\beta$ 1 (osteopontin / beta 1 growth factor) mediated by extracellular cells, matrix deposition and tubulointerstitial fibrosis, as well as its inhibition on myofibroblast epithelial tubular transdifferentiation. [9]

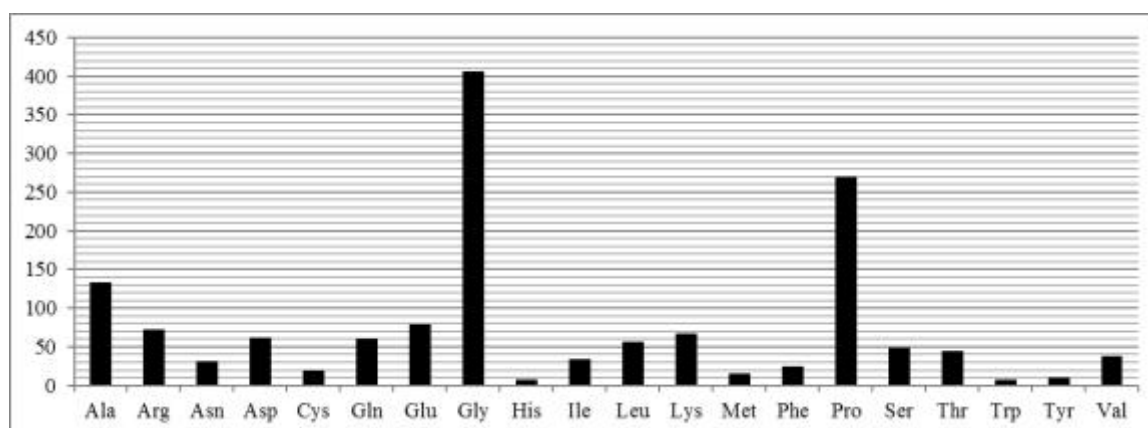


Fig.2: Graph of the amino acid content of human collagen.

Table.1: Calculation of the ETCs of the LEF in comparison with molecular oxygen and water.

No	Reducing agent	Oxidizing agent	HOMO	LUMO	BG	E-	E+	EP	ETC
1	O <sub>2</sub>	H <sub>2</sub> O	-10.733	4.059	14.792	-0.038	0.171	0.209	70.775
2	O <sub>2</sub>	LEF	-10.733	-0.484	10.249	-0.038	0.140	0.178	57.579
3	O <sub>2</sub>	O <sub>2</sub>	-10.733	-0.982	9.751	-0.038	0.138	0.176	55.403
4	H <sub>2</sub> O	H <sub>2</sub> O	-12.316	4.059	16.375	-0.127	0.171	0.298	54.950
5	H <sub>2</sub> O	LEF	-12.316	-0.484	11.832	-0.127	0.140	0.267	44.315
6	LEF	H <sub>2</sub> O	-9.246	4.059	13.305	-0.135	0.171	0.306	43.480
7	H <sub>2</sub> O	O <sub>2</sub>	-12.316	-0.982	11.334	-0.127	0.138	0.265	42.770
8	LEF	LEF	-9.246	-0.484	8.762	-0.135	0.140	0.275	31.862
9	LEF	O <sub>2</sub>	-9.246	-0.982	8.264	-0.135	0.138	0.273	30.271

The initiation and monitoring practices of rheumatologists in Australia using LEF were also evaluated. The choice of the initial dose of LEF among the Australian rheumatologists who responded varied considerably. [10] Other researchers studied the profile of side effects and survival characteristics of LEF used in a regional population of patients in New Zealand (NZ). They concluded that their studies suggest a better profile of side effects and better survival of the drug for LEF than

suggested by previous studies with a survival comparable to that of methotrexate.

## II. MATERIALS AND METHODS

We obtained the information about the collagen of "The National Center for Biotechnology" Information (NCBI): LOCUS CO2A1\_HUMAN 1487 aa linear PRI 10-OCT-2018 DEFINITION Rec Name: Full=Collagen alpha-1(II) chain; Alt Name: Full=Alpha-1 type II collagen;

Contains: Rec Name: Full=Collagen alpha-1(II) chain;  
 Contains: Rec Name: Full=Chondrocalcin; Flags:  
 Precursor. ACCESSION P02458 VERSION P02458.3  
 DBSOURCE Uni Prot KB: locus CO2A1\_HUMAN,  
 accession P02458; class: standard.

We obtained the formula of the LEF on the page of PubChem figure1.

In Figure 2 the graph is presented. You can see that Gly is the most abundant amino acid of all its structural composition; while Trp is the amino acid with fewer units.

In Table 1 it can be seen that the lowest value of ETC corresponds to the LEF-O<sub>2</sub> interaction; This means that the LEF is easily oxidized. It can also be seen that the LEF-H<sub>2</sub>O interaction is not as deep in the quantum well; this indicates that the LEF is not very soluble in water.

Table 2 shows the calculations of two new concepts. The quantum molecular impedance is relative to water (QMIRW) and the quantum molecular conductance relative to water (QMCRW). With these two concepts, the reader will better understand the concept of ETC.

We can observe in this table 2 that the LEF-O<sub>2</sub> interaction has almost half the value of the valence electron jump impedance of LEF towards O<sub>2</sub> than the jump of H<sub>2</sub>O to another molecule of H<sub>2</sub>O. With the conductance, the opposite happens.

The quantum calculations we carry out with the hyperchem software. These calculations were made in other articles already published by us. [11-15]

### III. RESULTS AND DISCUSSIONS

We characterize human glycogen with the software model 6000. [18] Information on the sequencing of this protein was taken from the NCBI database.

Table.2: Calculation of MQIRW and MQCRW.

This calculation is based on the ETCs in Table 1.

No	Reducin g agent	Oxidizin g agent	*MQIR W	**MQCR W
1	O <sub>2</sub>	H <sub>2</sub> O	1.288	0.776
2	O <sub>2</sub>	LEF	1.048	0.954
3	O <sub>2</sub>	O <sub>2</sub>	1.008	0.992
4	H <sub>2</sub> O	H <sub>2</sub> O	1	1
5	H <sub>2</sub> O	LEF	0.806	1.240
6	LEF	H <sub>2</sub> O	0.791	1.264
7	H <sub>2</sub> O	O <sub>2</sub>	0.778	1.285
8	LEF	LEF	0.580	1.725
9	LEF	O <sub>2</sub>	0.551	1.815

\*Molecular quantum impedance relative to water (MQIRW)

\*\*Molecular quantum conductance relative to water (MQCRW)

The QMIRW and the QMCRW should not be confused with traditional impedance and conductance.

These concepts are similar; but, not the same.

Table.3: This table shows the 13 most likely and strongest interactions of 40 calculated.

No.	Reducing agent	Oxidizing agent	HOMO	LUMO	BG	E-	E+	EP	ETC
13	LEF	Thr	-9.246	0.832	10.078	-0.135	0.191	0.326	30.914
12	LEF	Lys	-9.246	0.943	10.189	-0.135	0.195	0.330	30.875
11	LEF	Pro	-9.246	0.792	10.038	-0.135	0.191	0.326	30.791
10	LEF	Gln	-9.246	0.755	10.001	-0.135	0.192	0.327	30.584
9	LEF	Asn	-9.246	0.644	9.890	-0.135	0.193	0.328	30.153
8	LEF	Ser	-9.246	0.565	9.811	-0.135	0.198	0.333	29.462
7	LEF	Arg	-9.246	0.558	9.804	-0.135	0.199	0.334	29.353
6	LEF	Tyr	-9.246	0.293	9.539	-0.135	0.193	0.328	29.081
5	*LEF	*Glu	-9.246	0.438	9.684	-0.135	0.201	0.336	28.822
4	*LEF	*Met	-9.246	0.145	9.391	-0.135	0.192	0.327	28.719
3	*His	*LEF	-9.307	-0.484	8.823	-0.169	0.14	0.309	28.555
2	*LEF	*Asp	-9.246	0.420	9.666	-0.135	0.204	0.339	28.514
1	*Arg	*LEF	-9.176	-0.484	8.692	-0.165	0.14	0.305	28.499

\*These interactions are the five highest and strongest probability anchor points of the 41 calculated.

In Table 3, we can see the 13 interactions of 40 calculated. These 13 interactions show that only 2 of them

are oxidant and the other 11 are reductive. The five most reliable and most probable interactions of these are

indicated with one \*. Within these five interactions are the interactions of the LEF with His and Arg in oxidizing form. Therefore, these LEF interactions are the most dangerous because they are oxidants.

#### IV. CONCLUSIONS

In Table 4, we summarize the most significant interactions for LEF anchors in collagen amino acids.

Table.4: Summary of the most significant interactions.

Number	AA	Units	Percentages	
1	Ala	134	9.01%	Oxidative anchoring (1)
2	Arg	72	4.84%	
3	Asn	32	2.15%	
4	Asp	62	4.17%	Reductive anchoring (2)
5	Cys	19	1.28%	
6	Gln	60	4.03%	
7	Glu	79	5.31%	Reductive anchoring (5)
8	Gly	406	27.30%	
9	His	8	0.54%	
10	Ile	34	2.29%	Reductive anchoring (3)
11	Leu	56	3.77%	
12	Lys	67	4.51%	
13	Met	16	1.08%	Reductive anchoring (4)
14	Phe	25	1.68%	
15	Pro	270	18.16%	
16	Ser	48	3.23%	Minimun units
17	Thr	44	2.96%	
18	Trp	7	0.47%	
19	Tyr	10	0.67%	
20	Val	38	2.56%	
	Total	1487	100.00%	

The numbers placed in parentheses indicate their position in table 3.

The research hypotheses were fulfilled. Next they are enunciated with details.

Hypothesis 1: LEF interacts with collagen through its amino acids.

Yes, these 13 of 40 interactions (Table 3) show that only two of them are oxidant and the other 11 are reductive (antioxidant).

Hypothesis 2: LEF has a positive influence on arthritis.

According to hypothesis 1. Two of 40 Interactions are oxidants, 13 of the interactions that have the lowest ETC and high to medium probability are reducing (antioxidants). Therefore, it is concluded that LEF is more beneficial than malignant.

Hypothesis 3: Quantum chemistry determines the type of interaction of LEF with the amino acids of collagen.

Yes, all interactions were calculated using the hyperchem software using the SE-PM3 method.

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# Sample Design of the Interview about Gender Equality

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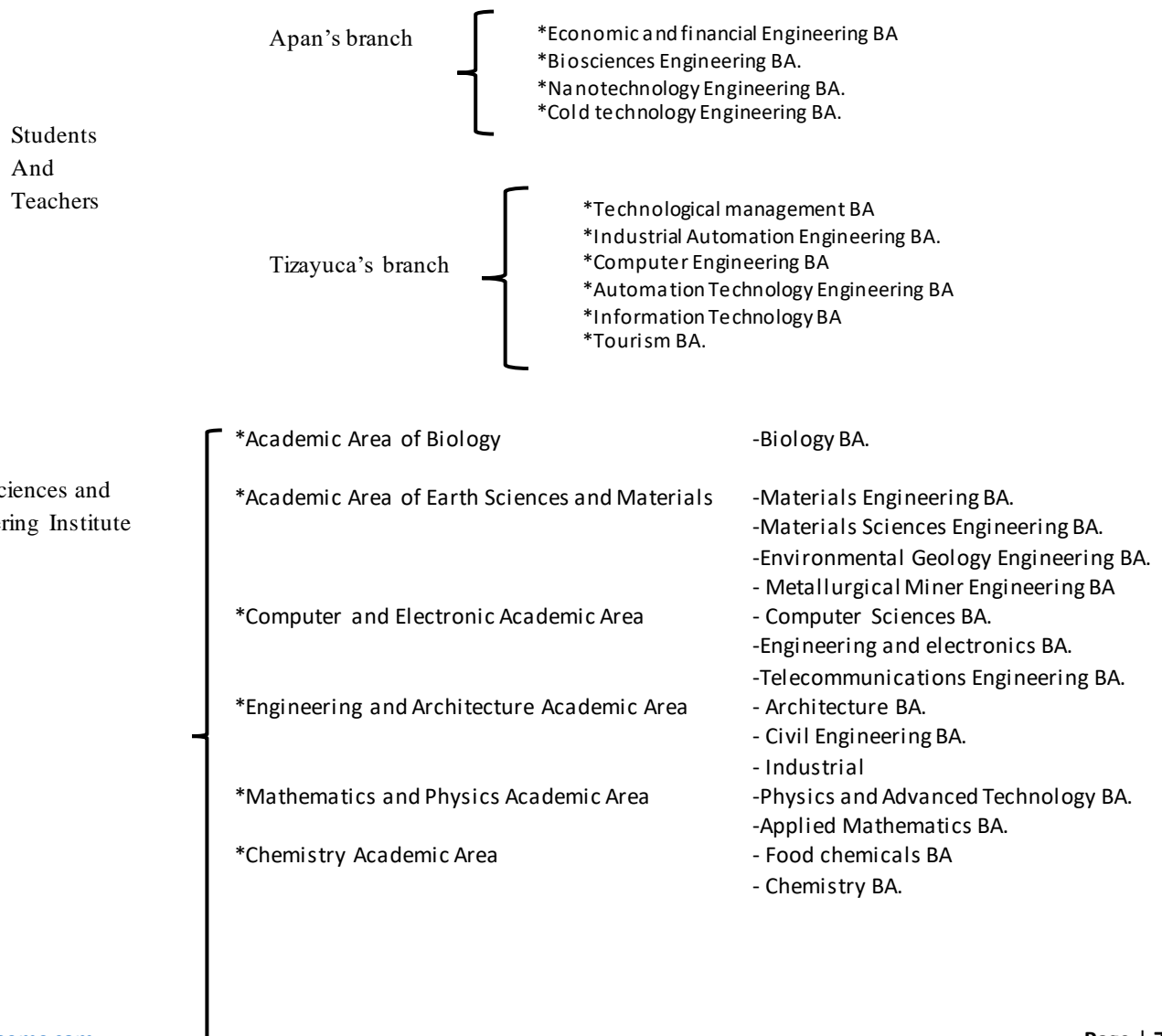
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## 1. SAMPLE'S OBJECTIVE

To determine the size of the students and academics population sample related to gender equality in the institutes and branches.

## 2. TARGET POPULATION

The study is oriented to the student's population with a higher level and full time and per academic hours in the following institutes and branches:



**SOCIAL SCIENCES  
AND HUMANITIES**

*Educative Sciences Academic Area	-Educative Sciences BA.
*Politic Sciences and Public Management Academic Area	-Politic Science and Public Management BA.
*Law and Jurisprudence	-Law BA
*History and Anthropology Academic Area - Social Anthropology	- Mexican History BA.
*Sociology and Demography Academic Area	-Regional Planning and Development BA.
*Social Working Academic Area	- Sociology BA.
*Communication BA.	- Social Working BA.
*Foreign Language Academic Area	- Communication BA.
	- Foreign Language BA.

### 3. SAMPLE RANGE

The sample is designed in order to give results about equality, an also about the gender violence and discrimination inside the Institutes and Branches in Universidad Autónoma del Estado de Hidalgo.

### 4. SAMPLE DESIGN

The sample design of this study is characterized by its probabilistic, so, the interview obtained results are generalized to the entire sample and are by order, because the last selected unit are the students and teachers that are enrolled in some BA. In the stratified sample, the population of N units is divided in subpopulations of N<sub>1</sub>, N<sub>2</sub>, N<sub>3</sub>.....N<sub>L</sub> units, respectively. These subpopulations are not overlapped and in their groups include all the population, so, (Cochran, 1977):

$$N_1 + N_2 + N_3 + \dots + N_L = N$$

The subpopulations are called stratum, to get all the benefits of this stratification, the values of the N<sub>b</sub> must be known. Once determined the stratum, a sample of each one is removed, the removals must be done independently in the different stratum. The sizes of samples in the stratum are denoted as n<sub>1</sub>, n<sub>2</sub>, n<sub>3</sub>, ..., n<sub>L</sub>

### 5. SAMPLE SETTING

The setting of the sample used related to a stratified sample, which is classified in the following way:

Stratum 1	Stratum 2	Stratum 3	Stratum 4
155 Economical and Financial Engineering BA. (2015) 107 Biosciences Engineering BA. (2015) 87 Nanotechnology Engineering BA (2015) 120 Cold Technology Engineering BA- (2012) 121 Technological Paperwork BA. (2009) 52 Industrial Automation Engineering BA. (2017) 136 Computer Engineering BA. (2010) 82Automation Technologies Engineering BA. (2010) 71 Information Technologies BA. (2017) 375 Turism BA. (2001) 587 Biology BA. (2004) 215 Materials Engineering (2013) 9 Materials Science Engineering BA. (Manufacturing) (2003) 4 Materials Science Engineering BA. (Nonmetallic materials) (2003) 384 Environmental Geology Engineering BA. (2004 -2016) 100Environmental Geology Engineering BA. (Plan 2004 Aplied Geology Engineering) (2004)			

[illegible]

Chart 1. Population Stratum  
Source. Personal making

## 6. ELEMENTAL UNITS FORMATION OF SAMPLE

The elemental units of sample are grouped in four events, related to the population that is formed by Institutes and Branches , so that, the sample remain in the following way:

-1<sup>st</sup> period: based in the last part, it is calculated the size of the sample, it must be representative of the target population in each BA. If we start of the case that the electoral cage is a simple random process, the size of the sample is determined through the following algebraic expression:

$$n_j = \frac{N_i * (Z_\alpha)^2 PQ}{e^2(N_i - 1) + (Z_\alpha)^2 PQ}$$

Where:

- $N_i$  is the size of the sample j –BA
  - $N_i$  is the size of the population j-BA
  - P is the amount of success response
  - Q is the amount in failure response
  - $Z_{\alpha}$  with a trust level of 0.95, its value will be 1.96
  - E is the highest mistake allowed that we are ready to make to M for a trust level of 95%. For this case, the highest failure allowed is 16%
- 2<sup>nd</sup> Period: once calculated the sample in each BA., we make the calculus of the sample size of each Institute and Branches, this calculus must be in the following way:



$$\sum_{j=1}^{n_j} n_j = n_i ; \text{ such that } i \neq j \text{ where } i \text{ and } j \text{ go from } 1, 2, 3, \dots, L$$

-3<sup>rd</sup> period: from second period on, it is calculated the sample size of students and teachers, it means:

$$n_D = \sum_{i=1}^{n_i} n_{Di} \rightarrow \text{sample Size for teachers}$$

Where:

$$n_{Hi} = n_i \left( \frac{N_D}{N} \right), \text{ where } N_D \text{ is the teachers population and } N \text{ is the full population}$$

$$n_A = \sum_{i=1}^{n_i} n_{Ai} \rightarrow \text{is the students sample}$$

Where:

$$n_{Ai} = n_i \left( \frac{N_A}{N} \right), \text{ where } N_A \text{ is the students population and } N \text{ is the full population}$$

Based in the last part, the sample size is stated in the following way:

Teacher	Student	STRATUM I		STRATUM II	STRATUM III	STRATUM IV
4	26	30	Economical and Financial Engineering BA. (2015)	Apan's Higher education School Tizayuca's Higher education school Basic Sciences & engineering' Institute	114 165 529	Students 114 Students Teachers
4	24	28	Biosciences Engineering BA. (2015)			
4	23	26	Nanotechnology Engineering BA (2015)			
4	25	29	Cold Technology Engineering BA- (2012)			
4	25	29	Technological Paperwork BA. (2009)			
3	19	22	Industrial Automation Engineering BA. (2017)			
4	25	30	Computer Engineering BA. (2010)			
3	22	25	Automation Technologies Engineering BA. (2010)			
5	21	34	Information Technologies BA. (2017)			
5	29	35	Turism BA. (2001)			
4	30	32	Biology BA. (2004)			
1	28	7	Materials Engineering (2013)			
1	6	4	Materials Science Engineering BA. (Manufacturing) (2003)			
5	3	34	Materials Science Engineering BA. (Nonmetallic materials) (2003)			
			Environmental Geology Engineering BA. (2004 -2016)			
			Environmental Geology Engineering			

4	29	27	BA. (Plan 2004 Applied Geology Engineering) (2004)	Social Sciences & Humanities' institute	351	162
5	24	35	Metallurgical Miner Engineering BA. (2010)			Teachers
			Computer Sciences BA. (2010)			
5	30	36	403 Electronics Engineering BA. (2010)			
5	31	34	Telecommunications Engineering BA. (2012)			
5	30	35	Architecture BA (2003)			
			Civil Engineering BA. (2010)			
5	30	36	Industrial Engineering BA. (2010)			
			Physics and Advanced Technology BA. (2004)			
5	31	36	Applied Maths BA. (2010)			
4	31	31	Chemical Food BA. (2000)			
4	26	32	Chemistry (2000)			
			Chemical Food BA. (2013)			
1	27	10	Education Sciences BA. (2000)			
5	9	34	Politic Sciences & Public			
5	29	34	Management BA. (2013)			
5	29	35	Politic Sciences & Public			
5	30	35	Management BA. (2005)			
3	30	18	Law BA. (2005)			
			Social Anthropology BA (2009)			
5	16	36	Mexican History BA. (2013)			
			Regional Planning and development BA. (2013)			
3	31	23				
4	20	29	Sociology BA. (2003)			
4	25	30	Sociology BA. (Culture Sociology) (2003)			
4	26	28	Social working BA. (2013)			
2	24	14	Communication BA.			
5	12	35	Foreign Language BA.			
5	30	36				
5	31	33				
	28					

Chart 2. Sample strata

Source. Personal making

## 7. Spread factors

The spread factor over P sample units of that random selection is made by the following expression:

$$fexp_{I(i)} = \frac{N_{(i)}}{n_{(i)}} \text{ for } i = 1, 2, 3$$

Where

\* $N_{I(i)}$ : students and teachers quantity

\* $n_{I(i)}$ : selected students and teachers quantity

Applying the previous part:

From the context in Institutes and Branches:

INSTITUTES AND BRANCHES	POPULATION	SAMPLE	SPREAD FACTORS
Apan's higher education Branch	469	114	4
Tizayuca's higher education Branch	837	165	5
Basic sciences & engineering Institute	7325	529	14
Social sciences & humanities Institute	3720	351	11

Chart 2. Sample stratum

Source. Personal making

The ability that each student and teacher has from the total population is the following:

\*In the Apan's higher education school each selected student and teacher in the sample has the ability to represent to 4 of them.

\*In Tizayuca's higher education school each selected student and teacher in the sample has the ability to represent to 5 of them.

\*In the Basic Sciences and Engineering Institute, each selected student and teacher in the sample has the ability to represent 14 of them.

\* In the Social Sciences and Humanities Institute, each selected student and teacher in the sample has the ability to represent to 11 of them.

From the context of students and teachers:

	POPULATION	SAMPLE	SPREAD FACTOR
Students	10582	998	11
Teachers	1769	162	11

The ability that each selected student and teacher has in the total population is 11 persons, it means, each selected student and teacher has the ability.

## 8. SAMPLE VIABILITY

To determine the sample's viability is very important that it is verified the sample's adjustment. Based in that part, we use the following algebraic expressions:

- Calculating the estimator the average show :

$$\bar{y}_{st} = \sum_{h=1}^4 W_h \bar{x}_h = \left(\frac{114}{1160}\right)(28.38) + \left(\frac{165}{1160}\right)(27.56) + \left(\frac{529}{1160}\right)(29.41) + \left(\frac{351}{1160}\right)(29.28)$$

So that:

$$V(\bar{x}) = \sum_h^L W_h^2 (1 - f_h) \frac{S_h^2}{n_h} = \left(\frac{114}{1160}\right)^2 \left(1 - \frac{114}{469}\right) \left(\frac{2.68}{114}\right) + \left(\frac{165}{1160}\right)^2 \left(1 - \frac{165}{837}\right) \left(\frac{18.07}{165}\right) + \left(\frac{529}{1160}\right)^2 \left(1 - \frac{529}{7325}\right) \left(\frac{1384}{529}\right) + \left(\frac{351}{1160}\right)^2 \left(1 - \frac{351}{3729}\right) \left(\frac{198.28}{351}\right)$$

Such that:

$$V(\bar{x}) = 0.00017 + 0.0017 + 0.505 + 0.047 = 0.554$$

\*The standard deviation of the amount:

$$Sd(\bar{x}) = \sqrt{V(\bar{x})} = \sqrt{0.553} = 0.744$$

\*The relative mistake of the sample

$$Cv(\bar{x}) = \frac{Sd(X_{st})}{X_{st}} = \frac{0.744}{28.99} = 0.026$$

\*The relative accuracy of the sample:

$$Pr = [1 - Cv(\bar{x})] * 100 = [1 - 0.026] * 100 = 97.4\%$$

Such precision is classified in the following way:

- $Pr \geq 95\% \Rightarrow$  a very good sample
- $90\% \leq Pr < 95\% \Rightarrow$  good sample
- $80\% \leq Pr < 90\% \Rightarrow$  suitable sample
- $Pr < 80\% \Rightarrow$  don't suitable

With a level of confidence of 0.95, with a level of significance of 0.05 and with a relative mistake of 2.6%, they can be sampled 1160 people, it reach a representation of 97.4% over the focus population.

\*Confidence interval to each stratum of the square:

$$\left[ \bar{x} \pm \left( Z_{\frac{\alpha}{2}} \right) \sqrt{V(\bar{x})} \right]$$

So that,

$$[28.98 \pm (1.96)\sqrt{0.553}] = [27.52 ; 30.44]$$

In total terms:

$$[1100.8 ; 1217.6]$$

With a level of confidence of 0.95 and a significance level of 0.05 the size of the sample can vary in 1101 to 1218 surveys.

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# The Role of Smart Personal Assistant for improving personal Healthcare

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**Abstract**— Machine learning is a subfield of computer science that evolved from the study of pattern recognition and computational learning theory in artificial intelligence. The focus of this paper is to improve personal healthcare using smart personal assistant which make use of the combination of machine learning and cloud. Making a doctor appointment through phone call is a tedious process and it may take more time. People who did not made the prior appointment have to wait on the queue which sometimes leads to dissatisfactions to the patients. To overcome this gap, smart personal assistant application is proposed using which users can get appointment of various doctors according to the current availability and at anytime and anywhere. This will improve time saving from patients' side as well as they will be satisfied by timely service.

**Keywords**— cloud service, healthcare, machine learning, smart personal assistant

## I. INTRODUCTION

Time plays a major role in everyone's life. We are in the digital era. We never want to wait to receive or buy anything if it takes more time. If the waiting time for obtaining any goods or products means we will be looking for a better any other option or chance so that we can receive our goods or products in a timely manner. Smart personal assistants (SPA) play a major role nowadays. People are now moving towards SPAs. The implementation of context-aware computing is possible via personal assistants known as User Assistance Systems, virtual agents or SPAs, such as Google Assistant, Amazon Alexa, Microsoft Cortana or Samsung Bixby [1]. There are considerable differences between them.

Maedche et al. suggested a classification based on two dimensions: i) the degree of intelligence of the system, ii) the degree of interaction implemented by the system. In contrast to basic systems characterized by a low degree of interaction and low degree of intelligence, advanced systems are characterized by more sophisticated features. They allow users to decide whether to follow the assistance, provide a high extent of context-aware and

proactive assistance, include adaptation capabilities, and detect users' needs [2].

Digital personal assistants in the form of chatbots offer a lot more than simple messaging apps. They can be voice controlled, which makes it possible to use them also when our hands are full with any other activities [3].

Nowadays people are more connected and in healthcare organizations also use new innovative technologies to improve patient care. Voice assistants and voice enabled devices also offer significant promise to increase patient engagement, improve outcomes and reduce cost. Most of the healthcare institutions are already using voice enabled intelligent devices to improve patients' healthcare.

## II. RELATED WORK

A personal digital assistant or handheld computer is a small, mobile, handheld device that provides computing and information storage/retrieval capabilities. Recent years have seen a significant increase in the deployment of voice-controlled personal digital assistants. Some of the example products are Apple's Siri, Google's Now and Nuance's Nina. Some of the improvements possible are: i) extended dialog history, ii) improved context awareness, iii) dynamic system adaptation, and, iv) supported task hierarchy design [4].

The use of speech recognition is increasing rapidly and is now available in smart TVs, desktop computers, every new smart phones, etc allowing us to talk to computers naturally. With the use in home appliances, education and even in surgical procedures accuracy and speed becomes very important [5].

The growth in Human-Computer interaction field has not only been in quality of interaction, it has also experienced different branching in its history. Instead of designing regular interfaces, the different research branches had different focus on the concepts of multimodality, intelligent adaptive interfaces rather than command or action based, and finally active rather than passive interfaces [6].

PDA's are used in various fields. A study [7] described the usage of PDA's among medical students are analysed. The

table below gives the application of PDAs for various factors by the students.

Table.1: Common uses of PDAs among medical students (n=53) [7]

S.No	Purpose	Number of students
1	Calendar	48
2	Use drug reference	41
3	Email/text	26
4	Clinical reference text	26
5	Dictionary	22
6	Perform clinical calculations	15
7	Access different diagnoses	13
8	Take notes	11
9	Access course information	10
10	Take pictures	9
11	Search for literature	3

A systematic review of surveys demonstrated that a PDA was more likely to be accepted and used among physicians and younger and those who were working in large and hospital-based practices. Although PDAs could not store or organize large graphics and patients' entire medical records, they have played a significant role in managing certain amount of electronic documentation and accessing it at the point of care easily. Using mobile technologies such as smart phones and tablets with high quality design investigating the effectiveness and efficiency of using mobile devices for specific tasks are needed [8].

### III. SYSTEM ARCHITECTURE

The objective of this work is to build an AI personal assistant that helps user to schedule doctor appointment to a specific doctor at any time and place. The users have to find easily the nearby hospitals and availability status of the doctor. If the user wishes to schedule the appointment they have to pick the time slot and instant confirmation have to be made. In case if the doctor cancelled the appointment, the user can pick any other doctor appointment time slot. Rescheduling of the appointment also provided to give more comfortable to the user. In addition to the appointment scheduling system this application keeps track of the health record with the ML program it keeps on notify the user regarding the timely visit to the doctor and also help them to take their medicine on time in daily basis. It includes speech recognition system which will be easier to the user to communicate with it. It supports major languages being spoken in India so that even the normal people can easily interact without any conflicts. This application can be integrated in Facebook messenger, Skype, Telegram,

Website, Kik and slack community. This application is also available for android and windows platform. This application is need not to be installed by the user. All Android 5.0+ devices is preinstalled with Google Action App. This personal assistant can be triggered by launching the Google Action and just saying the app name. The Google Action will get connected to our personal assistant and can be executed there. This is easy for people and do not having the problem of downloading the application and also space issue in their device.

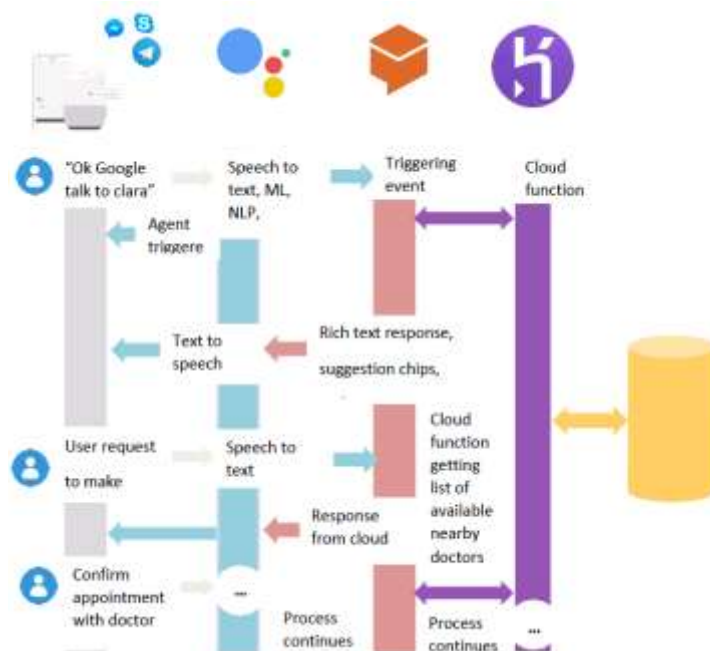


Fig. 1: System architecture

The dependencies used in this work to achieve our objective are given as follows:

1. Google Cloud Platform
2. Dialogflow
3. Heroku Cloud App Hosting

#### 1. Google Cloud Platform:

In this work, the features of NLP (Natural Language Processing), ML (Machine Learning) and APIs (Application programming interface) are used from Google Cloud Platform. NL API is a REST (Representational State Transfer) and consists of JSON requests and response. All requests from cloud are given in the form of JSON. ML part is used to train the application for voice recognition. APIs are used to generate user interface while interacting with the application.



Fig. 2: Retrieving Cloud data (request in JSON format)

## 2. DialogFlow:

The main important functions to be involved using Dialogflow is the support of intent flow, platform integration and training the agent. To train the agent, Intent is used. Intents are used to map user input to responses. The Dialogflow has three main steps namely: i) User giving input, ii) Dialogflow agent parsing that input and iii) Agent returning a response to the user.

## 3. Heroku Cloud App Hosting:

To perform cloud functions, database access and backend code deployment, Heroku is used. Heroku is a cloud platform as a service supporting several programming languages.

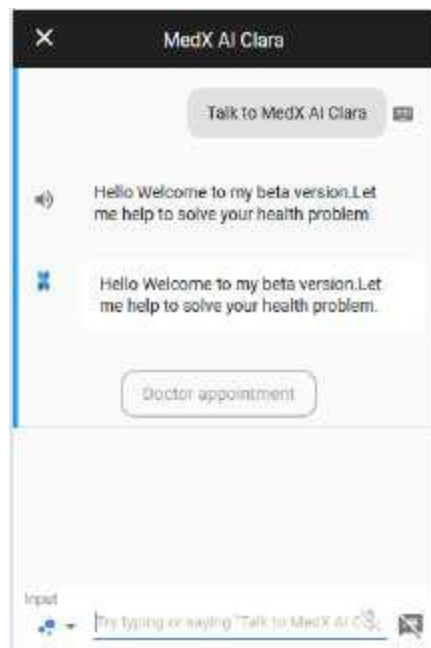


Fig. 3: MedX AI Clara interface

## IV. SYSTEM ANALYSIS

MedX AI Clara is the name of the application created. It is hosted and executed in cloud. First the interface of MedX AI Clara is shown in figure 3 below. The next selection is finding the doctor appointment. It is given in figure 4. Then we have to select which category of doctor we want to see i.e. neuro specialist or dentist, etc. After

giving proper category, we can get the details of the particular doctor and then we can fix the appointment using that interface itself.

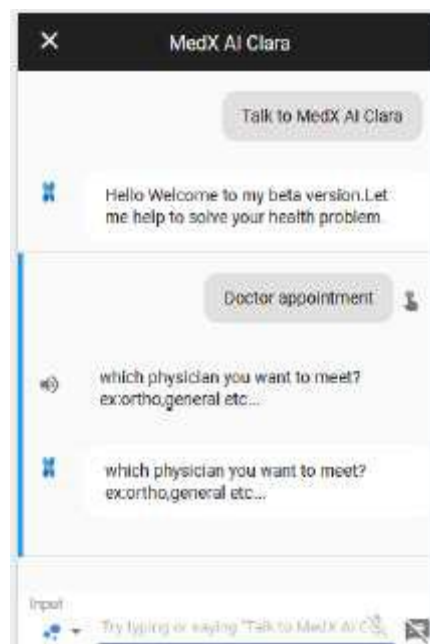


Fig. 4: Doctor appointment using MedX AI Clara

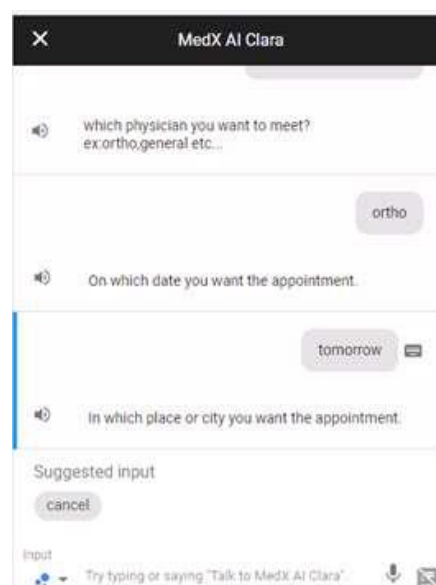


Fig. 5: Department selection & date using MedX AI Clara



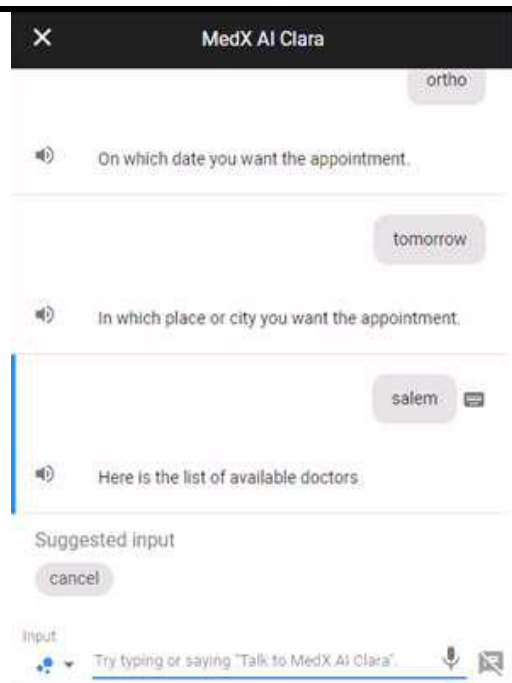


Fig. 6: Location selection using MedX AI Clara

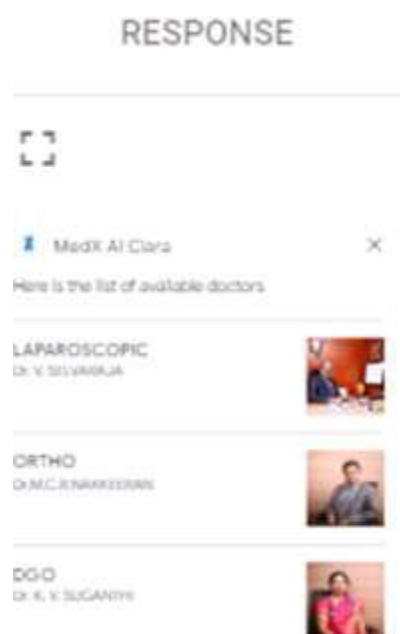


Fig. 7: Final response of available doctors using MedX AI Clara

## V. CONCLUSION

The proposed system provides quick confirmation of appointment. It also provides an easy interface and user can book appointment at any time with the doctor and at anywhere. Another advantage of using this system is people can book appointment in a short time and it also avail voice recognition feature to increase the speed of execution. Since everything is hosted in Cloud environment, the users need not to install the developed application in his/her smart device since everything is

hosted in cloud itself. If the device is capable of accessing Internet, then we can use this application anywhere which is smart enough since it reduces the time of interfacing for getting doctors appointment which is a time consuming process in traditional system practice. Also health is very essential factor and we have to get solution for the availability of doctors or specialists in emergency situation where we don't have enough time to talk and find the location and for appointment of those persons. This system will be helpful for people who have smart devices and who are in need of smart solution for their healthcare.

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# Proposal for the Creation of a Network of Family Businesses in the Mexican Coffee Industry

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**Abstract**— This article seeks to contribute to the union of Mexican coffee growers, growth and development of our coffee industry and increased commercial involvement by creating a network where family firms undertake strategic alliances, share and comply with standards of communication, technology, management information and knowledge, among others. Explanatory and descriptive documentary analysis of the importance of coffee farmer in Mexico category was performed in order to propose a Network model of Coffee in Mexico. The main pillars on which rests the network are: information, technology, knowledge and goods and services.

**Keywords**— coffee, family business, networks.

**Resumen**— Este artículo busca contribuir a la unión de los cafeticultores mexicanos, el crecimiento y desarrollo de nuestra industria cafetalera y una mayor participación comercial mediante la creación de una red donde las empresas familiares realicen alianzas estratégicas, compartan y cumplan con estándares de comunicación, tecnología, administración, información y conocimientos, entre otros. Se realizó un análisis documental explicativo y descriptivo sobre la importancia del rubro cafeticultor en México, para posteriormente proponer un modelo de Red del Café en México. Los principales pilares en los que descansa la red son la información, la tecnología, los conocimientos y los bienes y servicios.

**Palabras Clave:** café, empresas familiares, redes.

## I. INTRODUCTION

Coffee, source of many stories, legends and traditions, is a native beverage universally known, originating in Ethiopia

Africa that comes from a plant called coffee, of which there are several varieties in the world. Greater production worldwide is the family of the Arabian with 70 percent of production, this is followed by the robust, originating from Uganda and its main producer is Vietnam. To Mexico, coffee is the second product in volume of our exports, oil is number one. Brazil being the main producer (Almazara, 2012).

Today, the coffee industry is facing a very competitive and industrialized world, coffee being one of the main agricultural products consumed worldwide. Mexico is one of the leading producers of coffee, ranking sixth as a producer (Amecafe, 2012), thanks to national geography that allows cultivate and produce ranked among the world's best varieties, which are grown in twelve states of the Mexican Republic in an area of 688,718 hectares (Siap, 2010), Chiapas is still the main producer of this grain. Moreover, Mexico ranks first in the production of organic coffee.

Moreover, the production of coffee has ancestral population presented different problems of development and marginalization; its inhabitants, most of whom come from ethnic groups have suffered abuse and exploitation of third due to the lack of a more equitable for its handicraft and agricultural products trade process, as buyers and exporters who are governed by the laws of the local market for their products, this results in cheaper products.

It is for this that the coffee industry in Mexico, should updated, renew and be in constant innovation and development, in addition coffee producers need to organize themselves for the production and penetration into national and international markets in a better and greater way.

This article is intended to contribute to the growth and development of the coffee industry and the organization of producers of Mexican coffee through the identification of factors that allow these producers integrated into a system of enterprise network for improvement, promotion and development of coffee companies in Mexico and promote more and better participation of Mexican coffee industry in domestic and international markets. In-Network seeks that family businesses share and make strategic alliances, meet the standards of communication, technology, management, information, knowledge, goods and services and support each other for the growth of all members of the network.

This work consists of the introduction, description of coffee cultivation in Mexico, the theoretical framework, the results and conclusions.

Coffee cultivation in Mexico According to the Mexican Association of Coffee Production Chain AC Amecafe

demand / annual coffee consumption in the international context it is 134 million bags of 60 kg, while the supply / annual production is 133 million bags and 24 million bags of inventory. (Amecafe, 2014), so we notice that the market is very balanced.

For Mexico, according to figures from 2011-2012, as shown in Chart 1, the coffee is a strategic activity in the economic sphere; and employing more than 500,000 producers, about 690,000 hectares 12 states and 391 municipalities and involves Mexican exports 897,000,000 per year, making our country the leading producer of organic coffee in the world and destines 10 percent of its surface to this activity. In addition, coffee production directly and indirectly linked to nearly 3,000,000 people and generates a market value of about 20 billions pesos per year (Sagarpa, 2014).

**Chart 1**

### **Distribución de la Poducción de Café Convencional 2011.**

<b>% de la Superficie sembrada</b>	<b>Estados</b>
84	Chiapas, Veracruz, Oaxaca y Puebla
15	Guerrero, San Luis Potosí, Nayarit e Hidalgo
1	Jalisco, Querétaro y Tabasco

Fuente: [sagarpa.gob.mx](http://sagarpa.gob.mx).

The coffee production chain is one of the most important items in the agribusiness sector in the country, not only for its economic importance, but also the social and environmental impact generated. As mentioned above, the positioning of coffee both in the field of international market as in the domestic market is one of the strategic actions in the economic field for all involved in this system in coffee production. (See chart 2).

In Mexico, the coffee industry is mainly grouped in family enterprises, mainly in the agricultural part of the process,

not in the marketing or processing of the coffee cherry. It is in the process of agriculture, where it is important that its members have values, socialize smoothly and seek to achieve shared goals. That is, people with empathy, availability, perseverance, collaborating with the same objective, organized in family businesses are the ones most likely to succeed through an associative process, to join and share the results on a network or business consortium. (Vargas J. y Ticlla E, 2012).

**Chart 2**

### Datos Básicos del Cultivo del Café

	Concepto	U de M	Cantidad
	Superficie sembrada en 12 estados (miles)	Ha	760.4
	Superficie cosechada (miles)	Ha	687.7
	Composición de la superficie	%	97% arábigo y 3% robusta
<b>Producción</b>	Rendimiento (café cereza)	Ton/ha	1.86
<b>Nacional</b>	Producción anual de café cereza (miles)	Ton	1,285.80
<b>(2011/12)</b>	Sacos de café oro, beneficiado o verde de 60 kg	Miles	4,286.10
	Quintales de café oro, beneficiado o verde (45kg)	Miles	5,590.50
	Valor de la producción (millones)	\$	6,806.90
	Número de productores (80% zonas marginales, 66% indígenas)	Miles	542.20
	Productores de café orgánico	%	7
	Estacionalidad de la producción	%	El 66% se optiene de enero a marzo
	Quintales comercializados ciclo 2011/2012	Miles	2,524.80
	Exportación ciclo 2011/2012 (Miles)	Sacos de 60Kg	3,375.00
	Valor de exportación (millones)	Dólar/pesos	875.9/11,647.2
<b>Comercio</b>	Consumo per capita	kg/anales	1.43
	La composición porcentual de la exportación en:	café verde	76
		Industrializado	23
		Tostado y molido	1

Nota: El ciclo cafetalero es de octubre de un año a septiembre del siguiente

Elaborado con datos del SIAP, PNC, OIC y AMECAFE 2012.

Fuente: sagarpa.gob.mx

On the other hand, according to the Business Families Foundation (2013), Mexico is the fifth country with more family businesses in the world, generating these companies 90 percent of GDP and yet these are a vital part of the economy, facing a number of problems that limit their growth, maturation and permanency in the market, being the main ones the following.

- 70 percent of new businesses do not reach the third year of life.
- Do not have a succession plan.
- The recruitment is usually done with emotional and non-strategic bases
- Do not have a driving organ itself, eg a Board of Directors.
- There is no practice of monitoring budgets and business plans.

It is for this that according to Giovannuncci and Ponte (2010), in the current context of the global market, you can analyze the dynamics of sustainability in the coffee sector taking into account the role of different role players such as government and industry associations public and private, they constitute the regulatory framework in any specific sector. In this context, Bacon (2010) links the changes in world coffee markets with the opportunities and

vulnerabilities to sustain the livelihoods of farmers. The changes that characterize the crisis in conventional coffee markets are changing governance structures, corporate concentration, and oversupply of coffee bean and low prices. By contrast, certification of organic and fair trade is two alternative forms of trade and production of specialty coffees that can provide opportunities for small-scale producers.

Moreover, Palacios (2004), paying attention not only to the dynamics in the production and trade, but also the role of agents of mediation area, in this case the state agencies of different character, ensures that the influence expansion of global trade networks, under state protection in certain ecological-cultural<sup>1</sup>and despite its purported cultural authenticity niches are strategically in situations of dependence due to its roughly inferred monoculture of certain commercial products accession, as would be coffee. Another problem facing the coffee sector is the drastic reduction of government support for the sector, because as we can see in chart 3, support the productive promotion of

<sup>1</sup> Ecological-cultural niche is how an organism is related to their biotic and abiotic environment. In other words the niche is the role and the place of an organism in an ecosystem.

coffee has fallen in recent years compared to 2010, approximately 50 percent.

coffee producers benefit compared to 2010 is observed, as shown in chart 4.

As a result of reduced government support the productive promotion, an equally drastic reduction in the number of

### Chart 3

#### Apoyo a Fomento Productivo del Café 2007-2012

Monto Distribuido (pesos)

Entidad	2007	2008	2009	2010	2011	2012
Chiapas	162,816,740.50	181,562,919.50	189,527,424.00	176,726,967.69	68,351,783.64	103,874,139.38
Colima	906,596.00	560,677.50	1,061,838.00	1,106,875.83	409,824.70	524,660.94
Guerrero	20,714,923.50	25,611,743.00	28,407,998.00	27,590,988.90	13,417,513.77	15,389,488.14
Hidalgo	9,042,172.50	2,539,379.00	3,741,113.97	3,836,899.98	2,314,653.76	2,760,214.79
Jalisco	181,788.00	219,189.50	1,143,530.36	1,183,095.22	62,192.52	177,839.15
Nayarit	12,143,894.00	13,105,081.50	17,733,563.00	17,097,670.54	7,558,563.87	10,841,986.24
Oaxaca	73,220,460.00	85,720,354.00	93,890,889.34	88,164,244.04	36,850,474.29	44,298,043.90
Puebla	42,743,506.00	39,290,134.00	47,209,350.16	44,835,253.05	21,288,719.16	27,282,588.59
Querétaro	69,600.00	1,150.00	1,000.00	950.00	3,571.60	3,399.97
San Luis Potosí	4,287,025.50	6,103,960.50	7,038,938.04	7,187,544.45	3,043,898.59	2,774,643.53
Tabasco	316,150.00	650.00	650.00	617.50		
Veracruz	109,560,620.00	104,351,305.50	112,896,271.19	106,398,874.56	58,729,796.25	82,499,481.75
<b>Total</b>	<b>436,003,476.00</b>	<b>459,066,544.00</b>	<b>502,652,566.06</b>	<b>474,129,981.76</b>	<b>212,030,992.15</b>	<b>290,426,486.38</b>

Elaborado con datos del SIAP, PNC, OIC y AMECAFE

Fuente: sagarpa.gob.mx

Moreover, investment in research and development in the coffee sector reported a low level of activities of this type, while the lack of cooperation with the institutions that conduct research, development and innovation directly affects the competitiveness of studied sector (Becerra F. and H. Serna 2012).

It should be noted in this regard that the Secretariat of Agriculture, Livestock, Rural Development, Fisheries and Food (Sagarpa) has developed in recent years a particular program to encourage expenditure on research and development, it has called Procafe<sup>2</sup>, which announced a budget exercise for 2014 700,000,000 pesos. This resource aims to link producers with technological innovation in the development of infrastructure such as technologically advanced plants to mitigate the shortcomings caused by the existence of pests and the effects of climate change. This program links teamwork of producers, traders and scientists to find ways to help reactivate the coffee field.

<sup>2</sup> Procafe building program for agriculture which seeks to help increase production and productivity of agricultural rural economic units engaged in coffee cultivation in Mexico

Chart 4

### Apoyo a Fomento Productivo del Café 2007-2012

Número de Productores Beneficiados

Entidad	2007	2008	2009	2010	2011	2012
Chiapas	108,530	107,044	113,203	114,543	51,082	54,106
Colima	519	178	430	794	275	294
Guerrero	12,401	11,824	12,897	13,838	9,811	9,950
Hidalgo	24,585	2,112	3,125	3,952	2,541	2,360
Jalisco	536	30	180	258	36	60
Nayarit	3,167	2,997	3,942	6,599	2,427	2,497
Oaxaca	59,971	49,311	53,462	55,310	29,749	28,241
Puebla	29,439	27,129	30,547	30,747	17,728	15,060
Querétaro	217	1	1	1	8	8
San Luis Potosí	9,717	4,803	5,701	5,752	4,034	3,080
Tabasco	971	1	1	1	0	0
Veracruz	60,438	54,040	58,606	57,814	37,740	36,433
<b>Total</b>	<b>310,491</b>	<b>259,470</b>	<b>282,095</b>	<b>289,609</b>	<b>155,431</b>	<b>152,089</b>

Elaborado con datos del SIAP, PNC, OIC y AMECAFE.

Fuente: sagarpa.gob.mx

It is therefore important coffee growing internationalization of coffee Pymes, since programs are based on the construction of sectoral, regional and national competitiveness through the cooperative relationship between companies in the same industry, which are integrated to access projects with high risk, but essential for exploiting new markets through the development of activities to build a joint competitive strategy (Durán 2011). The coffee industry should be supported by institutions supporting enterprise networks formed with technical skills, reputation, legitimacy, neutrality and territorial presence; Also, for a regulatory framework conducive business environment, containing restrictions as conditions and consistent with external regulations.

Founded on the above, there are, according to the Ministry of Economy of the Mexican government; four main associations representing the coffee industry:

1. The Mexican Association of Coffee Production Chain (Amecafe). Emerges in 2006, in order to group the sectors involved in the agricultural process Emerges in 2006, in order to group the sectors involved in the agricultural, agro-industrial coffee processing; process from planting to retail

in the domestic and international market. Its mission is to make coffee growing so conducive to regional development and income generation for everyone in the chain profitable and sustainable.

2. The National Association of Coffee Industry AC (Canacafe). Founded in 1976 by a group of private companies. Today it involved 35 partners that manufacture and market instant coffee, roasted, ground and decaffeinated.
3. Coffees of Mexico. It was founded in 1985 as a channel of communication and liaison between all actors that are part of the coffee production chain. Report the outstanding activities at national and international coffee sector. Acts as the registration entity and select the topics of interest to the industry.
4. The Mexican Association of Coffee and Cafes AC Born in August 2004, its main function is to satisfy the needs of coffee bars, cafes and specialty coffee sector. Helps to find suppliers for goods, equipment, furniture, advice and training for a coffee shop. Boost coffee consumption in Mexico.



Note that each and every one of the above organizations plays a different role that often fails to complement a joint vision to maturity and sustainability of the sector on issues such as productivity, research and development and maturity enterprise networks that enable the positioning of the industry as one of the most important in Mexico.

## II. THEORETICAL FRAMEWORK

Regarding systemic structure of a network, it comprises three basic elements: nodes, which are the components (individuals, organizations, etc.) between which links of interest occur; relationships or exchanges of information, knowledge, technology, goods and services, etc., which essentially define and govern the behavior of the network; and finally communication, which can be determined by the (formal or informal) social roles played by nodes within the (Becerra, 2008) network.

According to Soto (2010), one of the research topics in the subject of coffee, is to evaluate the characteristics of the plant, since a more sustainable coffee system could be developed to better conservation of natural resources; this author argues that the relationship between the characteristics of the coffee plant has significant effects on production yields.

Venezuelan authors Narváez and Fernandez (2013) mention as to the Business Cooperation Networks<sup>3</sup>, the results indicate the formation of these is based on certain stocks comprising the relational dimension called *Social Capital*<sup>4</sup>. It also has as important factors promoting Social Capital, the fact that micro enterprises seen as key requirements for successful partner in a corporate network or consortium members possess values, socialize smoothly and ownership of shared goals. Is that people with empathy, availability, perseverance, and collaborating with the same goal are for micro-enterprises are more likely to succeed through an associative process. (Vargas and Ticlla 2012).

<sup>3</sup> Organizational structures, which consist of several companies, communicated and interrelated, to carry out joint projects without the need to create superstructures that would take them out individually.

<sup>4</sup> Social capital is an accounting term that is associated with the value of property or money that partners bring to a company without right of return

It also mentions that the traditional perspectives of social and economic development in the regions are giving way to more comprehensive views that include factors such as the interactions between agents, the peculiarity of the territories, cultural norms that govern human relations and the role that institutions can play. So that the promotion of social capital, in which the ability to form and nurture networking among regional actors, to foster a culture based on trust and cooperative values and strengthen effective institutions and policies and transparent included represents an important asset for achieving sustainable social development. (Rodriguez, 2012).

Another important aspect of enterprise networks reside in the institutions that support it, must comply with these technical skills, reputation, legitimacy, neutrality and territorial presence, accompanied by a regulatory framework conducive business environment and contains both constraints and conditions and consistency with external regulations. Mentioned as important external regulations dynamics of markets (government value chain), access to markets (dominant business strategy), patents, licenses, intellectual property, institutional environment and territorial, the sophistication of business strategy and access to productive factors and technologies. (Workshop Production Integration Projects Mif, Washington DC, October 2007).

As a family business, the essential elements that comprise are the property, business and family. With these elements one can say that the family business is one business organization in which ownership of the instrumental means and / or address are operationally in the hands of a group whose members family relationship exists. (Vélez, Holguín, De la Hoz and Duran, 2008).

Some other authors define the family business as one economic organization whose main purpose is the production or marketing of goods or services, and which are owned wholly or mostly a group of people united by family ties usually the descendants of the founder of it. (Thomas, 2008).

Family businesses as Gonzalo (2011) and Romero (2011) are the backbone of economic development, because in a market economy, the entrepreneur is the key. If there is no business, no company, no creation of jobs, no wealth creation.

## III. METHODOLOGY

To deepen this investigation the need to address it with the understanding that it is a reality in constant change (dialectical aspect) so the dialectical method is hereby

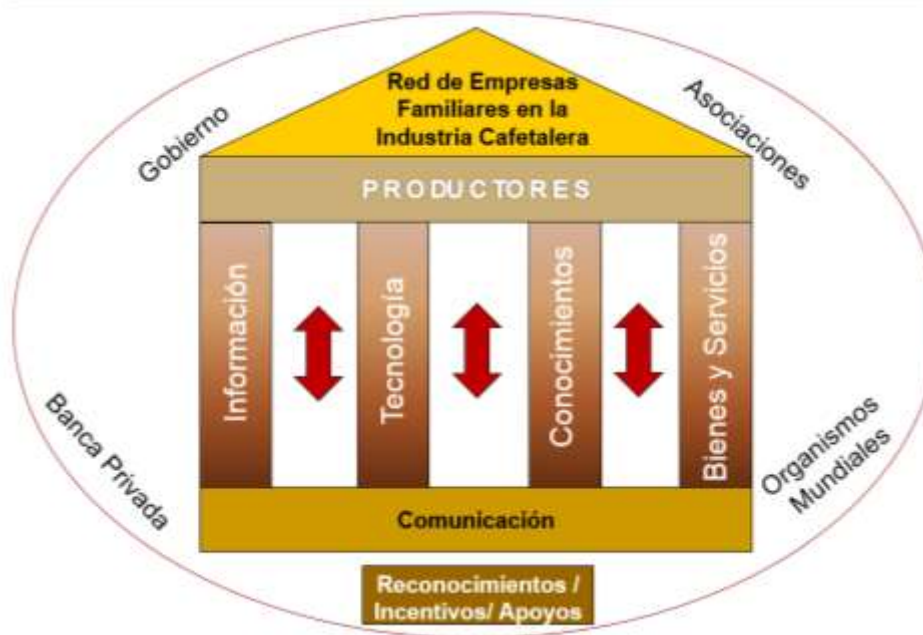


established. Moreover, there was the need based on existing theory, documentary research in libraries, databases and Internet, using national and international literature sources; Likewise, it was necessary to present a documentary analysis of the current role of family businesses in the coffee industry in Mexico and a documentary analysis of the model proposed in Red Coffee in Mexico, based on the variables of this. Finally, once the instruments of process analysis and interpretation of the information used, the

synthesis that would allow the establishment of conclusions (synthetic aspect) was performed.

#### IV. RESULTS

Then the diagram on the proposed establishment of the Network of Family Businesses in the Mexican coffee industry, allowing the union, the link and benefit to everyone involved is shown.



This proposal shows at the top of the familiares coffee companies that are producing party; they are supported in the foundation of communication holding four pillars. The first is information, where it is important that family businesses have databases that allow first instance those companies will create its history and statistics. Moreover, this information may be shared with others in the industry to make comparisons to identify best practices to be shared to benefit family businesses. The company information must be clear and concise so as to allow an auditable process.

As second pillar is the technology, which in this case can include a wide range of disciplines such as computer science, automation, robotics, pneumatics, electronics, and others. The notion of technology should be linked to all knowledge to make objects and modify the environment, intended to satisfy a need. Family businesses should have access to credit that allows them to purchase machinery and equipment. Especially in the processes that need to be optimized, such as family businesses often do not have sufficient capital to have an automated line. However, the proposed technology aims to get equipment to support

certain processes of the supply chain. For example, get the equipment to product packaging, pulping machine, toaster machine, etc.

Knowledge is a third pillar of family businesses, in which the expected contribution of the producers is to contribute to the network experience in their specific field and specialization of the production process for the production and marketing of coffee.

Finally, we have the pillar of goods and services, where importance is that the producer count in their home with at least the minimum infrastructure required for their production process and the state to provide basic services such so the producers to have this, improve their working conditions, they can be useful and will be reflected in improved productivity.

#### V. CONCLUSIONS

The creation of an enterprise network join the coffee production chain, as well as the main regulatory organizations, associations and twelve states leading coffee producers in Mexico, considering the common interests

with all these actors for increasing and improving the different stages of production and marketing of coffee.

Likewise, in the future family coffee companies could gain a competitive advantage as they have the support of a mature business network that offers a number of benefits that currently do not have, these are the benefits: Interact with business owners, b) Exchange of information and technology, c) Identify market opportunities, d) Permit be informed of the commercial, government and social events.

And besides, network will serve as a showcase for products of all members of coffee industry so if the network does have a structure of the proposal described in the results section, the company may have a demand orientation, an orientation towards the entrepreneur, business guidance and finally, an orientation to the generation of permanent changes in the production structure of entrepreneurs.

It is suggested as a complement to the success of the network, a review of the current context of government support to coffee producers, which is comprised of programs to support family businesses, organizations and associations in the coffee category that are created by the government.

It is suggested as a complement to the success of the network, a review of the current context of government support to coffee producers, which is comprised of programs to support family businesses, organizations and associations in the coffee category that are created by the government.

Also, conducting a Swot analysis in the sector in order to identify opportunities and weaknesses in the sector, to promote and implement new growth strategies, such as the fair trade and increasing certifications in products is suggested the increased production of organic coffee cultivation in Mexico which so far has the first place worldwide.

Continuously perform research and development in the sector and constant research of world markets, sending this information to coffee farmers through the proposed enterprise network. Overall emphasize the need for the corporate network is in constant awareness of the global environment, to continually circulate information, which may provide constantly updated to family coffee companies, for further growth of this industry.

All this adds up to ensure sustainable economic growth strategy to help raise growth rates of income and output per capita coffee producing regions, making conditions conducive to improving the quality of life of farmers, reducing poverty and preserving natural resources when growing coffee.

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# Demonstration of the Formation of the Caffeine-Dichloromethane-water Emulsion using Quantum Chemistry

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**Abstract**— Researchers have been concerned with the subsequent study of caffeine extraction. The objective of this article was to demonstrate how the caffeine-dichloromethane-water emulsion is formed. We use the theory of the electron transfer coefficient (ETC) as the cornerstone of our research. All the simulations of the interactions of the substances involved were calculated with the hyperchem simulator. The emulsion is formed because the  $ETC = 36,196$  of the caffeine- $CH_2Cl_2$  interaction is the lowest of the cross-band interactions of the mixture. It will expect massive amounts of caffeine emulsified with  $CH_2Cl_2$  and water. In conclusion, the gravitational well and the quantum well of caffeine coincide in being the lowest of all the wells calculated. It means that both  $CH_2Cl_2$  and  $H_2O$  will not destroy caffeine. That is, caffeine will be kept as a pure substance even after extraction with these two solvents. Although  $CH_2Cl_2$  extracts more caffeine, due to its low ETC, the product for human consumption can be contaminated.

**Keywords**— Caffeine, Dichloromethane, Water, Emulsion, Quantum Chemistry

## I. INTRODUCTION

Researchers have been concerned with the subsequent study of caffeine and catechins in the biomass of green tea using an optimized SFE (supercritical fluid extraction) method. The SFE of caffeine was carried out at different pressures (10, 20, 25, 30 MPa), temperature (30, 40, 50, 60 ° C) and extraction periods (1, 2, 3, and five h) for 10 g of sample. Caffeine extract yields and purity were optimized for successful separation. Optimal conditions for the extraction of caffeine were 25 MPa of pressure at 60 ° C for three h of extraction period. [1-3]

In other experiment investigators extracted caffeine with  $CHCl_3$  from the aqueous solution obtained by treating guarana powder with HCl, followed by filtration and alkalization. Using the melting point and thin layer

chromatography, they verified the purity of the isolated caffeine. [4]

A sequential statistical mixture allowed the optimization of extraction systems and mobile phase solvents to increase the differences detected in the metabolites of plants. [5-9]

The objective of this article was to demonstrate how the caffeine-dichloromethane-water emulsion is formed using calculations made with the hyperchem simulator.

## II. MATERIALS Y METHODS

We use the theory of the electron transfer coefficient as the cornerstone of our research. All the simulations of the interactions of the substances involved were calculated with the hyperchem simulator. We use the semi-empirical method PM3 specifically.

It has used this methodology in many projects carried out and published. [10-16]

## III. RESULTS AND DISCUSSIONS

Table 1 shows an extract from table 2. It shows the ETCs of pure substances in descending form according to the depth of the quantum wells. It can be noted that caffeine is the most stable substance of all because it is in the deepest well.

Table 1. ETCs of pure substances

Number	Reducing agent	Oxidizing agent	ETC
1	$CH_2Cl_2$	$CH_2Cl_2$	76.048
2	$H_2O$	$H_2O$	54.950
3	Caffeine	Caffeine	31.933

These ETCs were extracted from table 2 (below)

Table 2 shows all the possible interactions taken from two in two of these three pure substances. Interaction 9 has an  $ETC = 31.933$ . This value is the lowest of the nine

calculated interactions and tells us that caffeine is the most stable substance.

The other interactions are given according to their depth in the quantum well; they increase their instability until they reach the number  $\text{CH}_2\text{Cl}_2\text{-H}_2\text{O}$ . The most unstable substance is the substance with the highest energy.

Figure 1, shows us the difference between the ETC of  $\text{CH}_2\text{Cl}_2$  and caffeine is 44.115 units of ETC. The  $\text{CH}_2\text{Cl}_2$  is unstable; moreover, it falls to the bottom of the caffeine well and rises to it forming a new interaction of 4.263 units above. This new Caffeine- $\text{CH}_2\text{Cl}_2$  interaction has an ETC of 36.196. In this new interaction,  $\text{CH}_2\text{Cl}_2$  remains as an oxidizing agent of caffeine.

The different interaction was calculated, where caffeine is an oxidizing agent; ETC = 67.721. Because nature always seeks the least energy,  $\text{CH}_2\text{Cl}_2$  is more likely to be the oxidizing agent. The zone in which the two interactions of  $\text{CH}_2\text{Cl}_2\text{-Caffeine}$ , Caffeine- $\text{CH}_2\text{Cl}_2$ , are located is of average probability. That is, they do not go beyond the limits of their pure substances

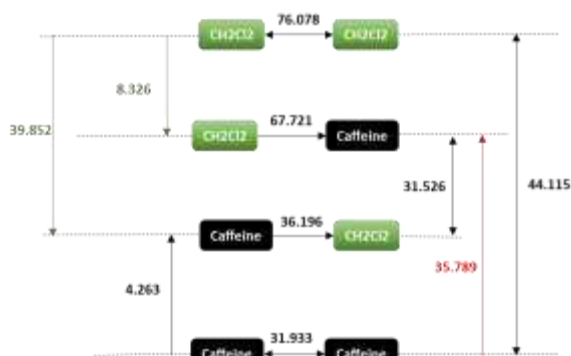


Fig. 1 Measures of the ETCs of the quantum well of the interaction caffeine and  $\text{CH}_2\text{Cl}_2$ .

Figure 2, show us the difference between the ETC of  $\text{H}_2\text{O}$  and caffeine is 23.017 units of ETC. As  $\text{H}_2\text{O}$  is unstable, it drops to the bottom of the caffeine well and rises it forming a new interaction of 11.087 units above. This new Caffeine- $\text{H}_2\text{O}$  interaction has an ETC of 43.019. In this new interaction,  $\text{H}_2\text{O}$  remains as an oxidizing agent of caffeine.

The different interaction was calculated, where caffeine is an oxidizing agent; ETC = 45.479. Because nature always seeks the lowest energy, that is, the deepest well,  $\text{H}_2\text{O}$  is more likely to be the oxidizing agent. The zone in which the two  $\text{H}_2\text{O}$  interactions-Caffeine, Caffeine- $\text{H}_2\text{O}$  are located is of medium probability. That is, they do not go beyond the limits of their pure substances.

By the way, we describe the two solvents and their interactions with caffeine; because the interaction pattern is identical, only the ETC values change.

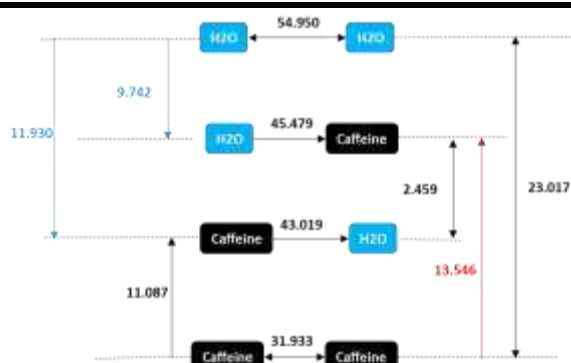


Fig. 2 Measures of the ETCs of the quantum well of the interaction caffeine and water.

In Figure 3, a different pattern of the  $\text{H}_2\text{O-CH}_2\text{Cl}_2$  mixture can be observed. In this case, the  $\text{H}_2\text{O-CH}_2\text{Cl}_2$  interaction has the lowest ETC. In contrast, the inverse interaction goes out of the upper limit. Therefore, the  $\text{CH}_2\text{Cl}_2\text{-H}_2\text{O}$  interaction falls in the area of least or nil probability. With these observations we can launch two hypotheses.

H1 " $\text{CH}_2\text{Cl}_2$  is an oxidizing agent of  $\text{H}_2\text{O}$ .  $\text{H}_2\text{O}$  cannot be an oxidizing agent of  $\text{CH}_2\text{Cl}_2$ ."

H2 " $\text{CH}_2\text{Cl}_2$  highly soluble in water"

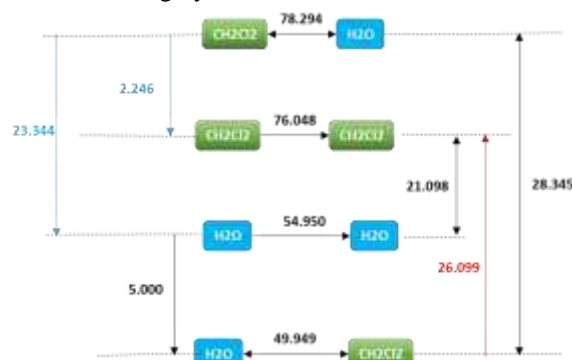


Fig. 3 Measures of the ETCs of the quantum well of the interaction dichloromethane and water.

We went to the laboratory to check our hypothesis. We find some controversies.

In Figure 4, a mixture of caffeine +  $\text{CH}_2\text{Cl}_2$  +  $\text{H}_2\text{O}$  is shown. In it, an unexpected emulsion is observed. The first time the emulsion is very homogeneous. In the second moment, it was left to rest, and two distinct phases were observed.

The bottom phase has an emulsion, and in the upper part, only a caffeine solution with water is shown.

We made a mixture of  $\text{H}_2\text{O-CH}_2\text{Cl}_2$  shown in figure 5. In this figure, it can be seen that the  $\text{CH}_2\text{Cl}_2$  was located at the bottom of the flask and the  $\text{H}_2\text{O}$  above. This phenomenon occurs due to the gravitational field since  $\text{CH}_2\text{Cl}_2$  is heavier than  $\text{H}_2\text{O}$ .





Fig. 4  $\text{CH}_2\text{Cl}_2 + \text{H}_2\text{O} + \text{Caffeine}$ . A) Freshly stirred mixture. B) Relaxed mix

Hypothesis 2 is not fulfilled. There is no solution; there are two phases in the flask. With this observation, it can be said that the gravitational well predominated over a quantum well. However, due to the lower ETC of the  $\text{H}_2\text{O}-\text{CH}_2\text{Cl}_2$  interaction, the interface of this mixture is powerful.



Fig. 5 Mixture of  $\text{H}_2\text{O} + \text{CH}_2\text{Cl}_2$

Why an emulsion?

The emulsion is formed because the  $\text{ETC} = 36,196$  of the caffeine- $\text{CH}_2\text{Cl}_2$  interaction is the lowest of the cross-band interactions of the mixture. Expect copious amounts of caffeine emulsified with  $\text{CH}_2\text{Cl}_2$  and water. In other words, caffeine is entrained by the  $\text{CH}_2\text{Cl}_2$  at the bottom of the flask due to the molecular weight of both. They do not separate due to their lower ETC of the crossed bands (Table 3).

In contrast, the  $\text{CH}_2\text{Cl}_2-\text{H}_2\text{O}$  interaction has a lower ETC of its binary mixture. Therefore, it also sticks to caffeine forming a trio. It can be said that the caffeine molecule acts as an emulsifying agent (or coupling agent) of  $\text{CH}_2\text{Cl}_2$  and  $\text{H}_2\text{O}$ .

Why Caffeine- $\text{H}_2\text{O}$  solution?

The  $\text{ETC} = 43,019$  is the lowest of the caffeine mix with  $\text{H}_2\text{O}$  traps caffeine in the water. They are located above the emulsion due to the molecular mass of the interaction.

Table 3. Quantum well (ETC) and gravitational well (Total mass)

Number	Reducing agent	Oxidizing agent	ETC	Total mass
1	$\text{CH}_2\text{Cl}_2$	$\text{H}_2\text{O}$	78.294	102.933
2	$\text{CH}_2\text{Cl}_2$	$\text{CH}_2\text{Cl}_2$	76.048	169.866
3	$\text{CH}_2\text{Cl}_2$	Caffeine	67.721	279.123
4	$\text{H}_2\text{O}$	$\text{H}_2\text{O}$	54.950	36
5	$\text{H}_2\text{O}$	$\text{CH}_2\text{Cl}_2$	49.949	102.933
6	$\text{H}_2\text{O}$	Caffeine	45.479	212.19
7	Caffeine	$\text{H}_2\text{O}$	43.019	212.19
8	Caffeine	$\text{CH}_2\text{Cl}_2$	36.196	279.123
9	Caffeine	Caffeine	31.933	388.38

#### IV. CONCLUSION

The gravitational well and the quantum well of caffeine coincide in being the lowest of all the wells calculated. It means that both  $\text{CH}_2\text{Cl}_2$  and  $\text{H}_2\text{O}$  will not destroy caffeine. That is, caffeine will be kept as a pure substance even after extraction with these two solvents ( $\text{ETC} = 33,933$ ). On the other hand, due to its mass and the gravitational well, the caffeine will precipitate in any of the solvents.

Although  $\text{CH}_2\text{Cl}_2$  extracts more caffeine, due to its low  $\text{ETC} = 36,196$ , the product for human consumption can be contaminated.

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Table 2. Cross-band ETCs of the 3 compounds involved in this investigation. These ETCs are ordered from highest to lowest according to the depth of your quantum well.

Number	Reducing agent	Oxidizing agent	HOMO	LUMO	BG	E-	E+	EP	ETC
1	CH <sub>2</sub> Cl <sub>2</sub>	H <sub>2</sub> O	-10.582	4.059	14.641	-0.016	0.171	0.187	78.294
2	CH <sub>2</sub> Cl <sub>2</sub>	CH <sub>2</sub> Cl <sub>2</sub>	-10.582	0.521	11.103	-0.016	0.130	0.146	76.048
3	CH <sub>2</sub> Cl <sub>2</sub>	Caffeine	-10.582	-0.491	10.091	-0.016	0.133	0.149	67.721
4	H <sub>2</sub> O	H <sub>2</sub> O	-12.316	4.059	16.375	-0.127	0.171	0.298	54.950
5	H <sub>2</sub> O	CH <sub>2</sub> Cl <sub>2</sub>	-12.316	0.521	12.837	-0.127	0.130	0.257	49.949
6	H <sub>2</sub> O	Caffeine	-12.316	-0.491	11.825	-0.127	0.133	0.260	45.479
7	Caffeine	H <sub>2</sub> O	-8.890	4.059	12.949	-0.130	0.171	0.301	43.019
8	Caffeine	CH <sub>2</sub> Cl <sub>2</sub>	-8.890	0.521	9.411	-0.130	0.130	0.260	36.196
9	Caffeine	Caffeine	-8.890	-0.491	8.398	-0.130	0.133	0.263	31.933