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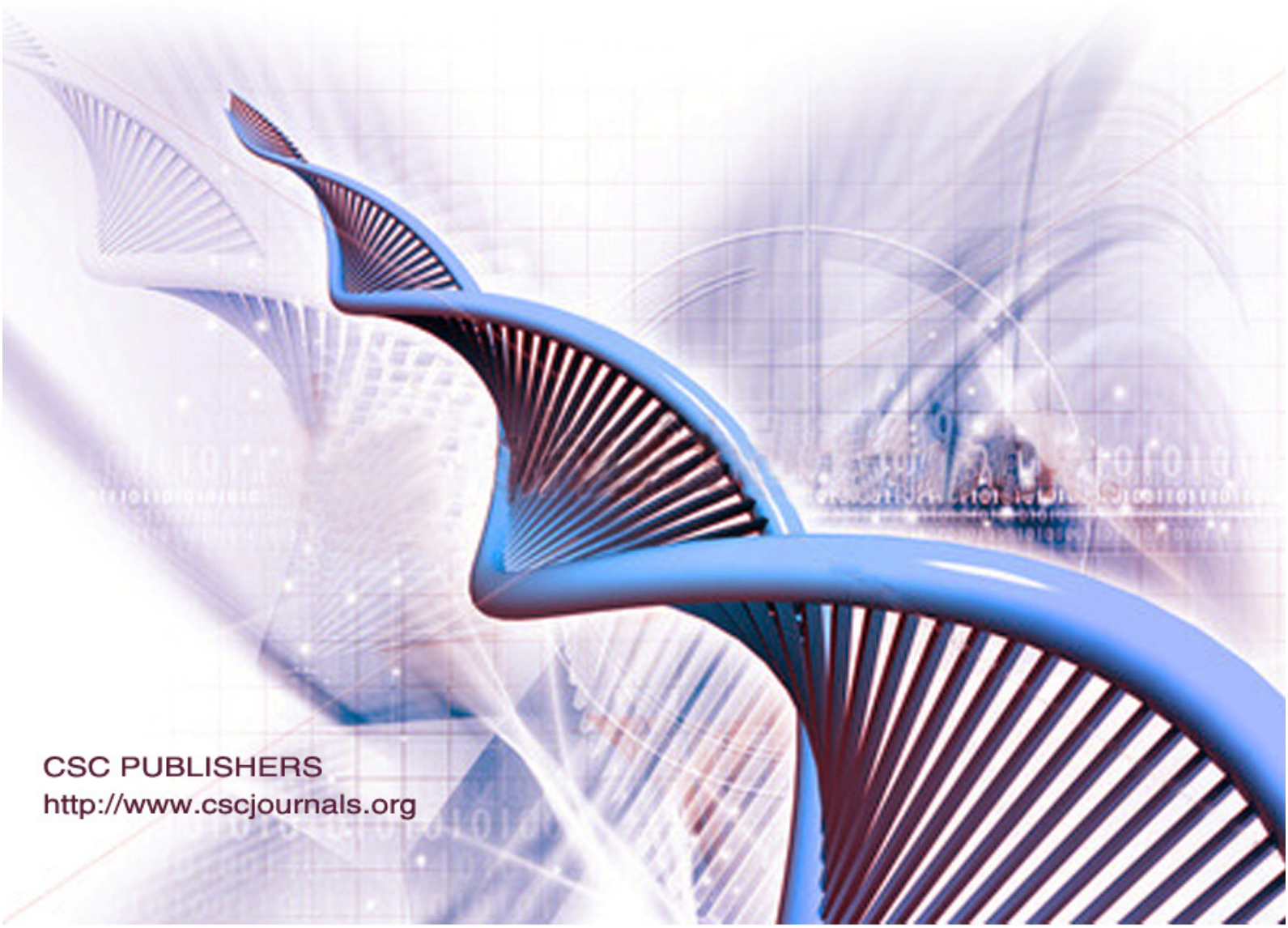

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**DR. NABEEL TAHIR**

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# EDITORIAL PREFACE

This is the fifth issue of volume five of International Journal of Biometric and Bioinformatics (IJBB). The Journal is published bi-monthly, with papers being peer reviewed to high international standards. The International Journal of Biometric and Bioinformatics is not limited to a specific aspect of Biology but it is devoted to the publication of high quality papers on all division of Bio in general. IJBB intends to disseminate knowledge in the various disciplines of the Biometric field from theoretical, practical and analytical research to physical implications and theoretical or quantitative discussion intended for academic and industrial progress. In order to position IJBB as one of the good journal on Bio-sciences, a group of highly valuable scholars are serving on the editorial board. The International Editorial Board ensures that significant developments in Biometrics from around the world are reflected in the Journal. Some important topics covers by journal are Bio-grid, biomedical image processing (fusion), Computational structural biology, Molecular sequence analysis, Genetic algorithms etc.

The initial efforts helped to shape the editorial policy and to sharpen the focus of the journal. Starting with volume 5, 2011, IJBB appears in more focused issues. Besides normal publications, IJBB intend to organized special issues on more focused topics. Each special issue will have a designated editor (editors) – either member of the editorial board or another recognized specialist in the respective field.

The coverage of the journal includes all new theoretical and experimental findings in the fields of Biometrics which enhance the knowledge of scientist, industrials, researchers and all those persons who are coupled with Bioscience field. IJBB objective is to publish articles that are not only technically proficient but also contains information and ideas of fresh interest for International readership. IJBB aims to handle submissions courteously and promptly. IJBB objectives are to promote and extend the use of all methods in the principal disciplines of Bioscience.

IJBB editors understand that how much it is important for authors and researchers to have their work published with a minimum delay after submission of their papers. They also strongly believe that the direct communication between the editors and authors are important for the welfare, quality and wellbeing of the Journal and its readers. Therefore, all activities from paper submission to paper publication are controlled through electronic systems that include electronic submission, editorial panel and review system that ensures rapid decision with least delays in the publication processes.

To build its international reputation, we are disseminating the publication information through Google Books, Google Scholar, Directory of Open Access Journals (DOAJ), Open J Gate, ScientificCommons, Docstoc and many more. Our International Editors are working on establishing ISI listing and a good impact factor for IJBB. We would like to remind you that the success of our journal depends directly on the number of quality articles submitted for review. Accordingly, we would like to request your participation by submitting quality manuscripts for review and encouraging your colleagues to submit quality manuscripts for review. One of the great benefits we can provide to our prospective authors is the mentoring nature of our review process. IJBB provides authors with high quality, helpful reviews that are shaped to assist authors in improving their manuscripts.

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# Enhancement of Multi-Modal Biometric Authentication Based on IRIS and Brain Neuro Image Coding

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**Abstract**

The proposed method describes the current forensics and biometrics in a modern approach and implements the concept of IRIS along with brain and resolves the issues and increases the strength of Digital Forensics Community. It has enormous features in biometrics to enhance diverse security levels. A new method to identify individuals using IRIS Patterns with the brain wave signals (EEG) is proposed. Several different algorithms were proposed for detecting, verifying and extracting the deterministic patterns in a person's IRIS from the Eye. The extracted EEG recordings form the person's brain has proved to be unique. Next we combine EEG signals into the IRIS patterns a biometric application which makes use of future multi modal combination architecture. The proposed forensic research directions and argues that to move forward the community needs to adopt standardized, modular approaches for person identification. The result of each authentication test is compared with the user's pre-recorded measurements, using pattern recognition methods and signal-processing algorithms.

**Keywords:** Electrodes, Electroencephalography (EEG), Neuro Image Coding, IRIS Patterns & Brain Waves, Signal Processing.

## 1. INTRODUCTION

Neuro image coding is a concept of capturing the specific data from IRIS and the brain matches with the database confidentially. Biometric system consists of uniquely recognizing a person based upon one or more independent physical or behavioral characteristics [1]. Identity access management and access control are two major roles in the bio-metric system. Verification and identification are two major functional parts.

In verification mode the system performs a one to one comparison of the captured patterns with already stored database templates. In Identification the system performs a one to many comparisons with templates and produces the result may be positive or negative recognition [1], [2]. The biometric system is more complex so that it cannot be violated. But sometimes it is more expensive and requires more software and hardware resources. When a new authentication system is implanted, it is essential a judgment between simplicity, price and efficiency, as well as social acceptability [1], [2]. When a new authentication system is implanted, it is essential a judgment between simplicity, price and efficiency, as well as social acceptability [1], [2]. The Digital forensics communities present in these times are not at the satisfied level. Even though we use the Biometrics methods for identify and access controls in a confidential manner, the security lacks.

*Unique Identification Authority of India (UIDAI) requires to connecting 2.4 Million eyes for Person Identification using IRIS biometrics in INDIA within five years.*

The Existing biometrics community are hurdled with privacy and discrimination, cancelable biometrics, danger to owner of secured items and spoofing. The finger prints of people who work in chemical industries are sometimes diminished. The voice of people may change if they have pneumonia or bronchitis, illness, fatigue, pitch, surgery involving tampering with the vocal cord, or any combinations of them. Age can also cause changes in the voice. If the surrounding area is noisier this kind of identification cannot be foolproof. In the DNA molecular structures of only a few people have been identified at present. It will take enormous effort and time to identify to find out the type of DNA of people all over the world [1]-[3].

EEG signals of each individual differs they are not same even if they do the same work or task [5], [6]. The brain of each individual is unique our DNA and our life expressions will certainly have an impact on our brain structure. It can be said that even if the DNA of two persons are the same their life experiences will differ [4]-[6]. When even security is needed we can use this brain biometric in access control systems. Since it is unique now a days biometrics are used in access control systems to gain access to resources protected from everyone except you. We leave our finger prints everywhere which can be replicated and used to gain access to any security information. But no one can gain access to the brain structure because it is safely protected inside the skull. Our brain activities are changeable.

A test was conducted the brain waves were interpreted and recorded from 200 subjects by think simply the password. The results were analyzed brain signals shows that everyone's brain waves are a bit difference even when they think about the same thing from brain waves we can authenticate users it produced 95% success rate [5], [6]. But later it is proved that the recorded signals are integration of gamma activity which is related to IRIS and muscular movement of eye. IRIS is a protected internal organ and has cells that are directly connected to the brain. So the integration of IRIS and Brain wave signals (EEG) recognition biometric systems to become the leading technology in identity verification. This work deals with the basic research in the field of the person identification by means of IRIS and Brain wave signals (EEG) [15], [16].

Our future work is mainly focused to the analysis of personal EEG features, suitable feature extraction algorithms, other parameterizations as well as classification techniques in Both IRIS Patterns and Brain wave signals (EEG), The detailed analysis of the EEG database and Fusion technique with clear strategies. We started Experimental study with the verification of results published in our further extension.

## 2. PROPOSED MODEL

Biometric Sensors used to capture the specific patterns from the IRIS and Brain wave signals (EEG) matches with the database confidentially. IRIS recognition uses pattern recognition techniques based on the irides of an individual's eye.

IRIS images are printed using a commercial printer and then presented at the IRIS sensor which is accepted and its identification can be duplicated. Since only alive people can make Brain wave signals (EEG), which is natural candidate for liveness detection it gives Anti Spoofing system design in existing unimodal IRIS biometrics.

The IRIS is the area of the eye where the pigmented or colored circle, usually brown or blue, rings the dark pupil of the eye [7], [8]. It includes the use of various techniques to either directly or indirectly images the structure, function or pharmacology of the brain.

A characteristic property of neuro imaging data is that they are acquired, processed and stored in digitized form. Without a clear strategy for enabling research efforts bio metrics build upon one another, but it will fall behind the market. In order to rectify this problem a new approach is suggested. Neuro Image Coding makes it possible that data processing, data analysis and data interpretation can be done on IRIS with Brain wave signals (EEG).

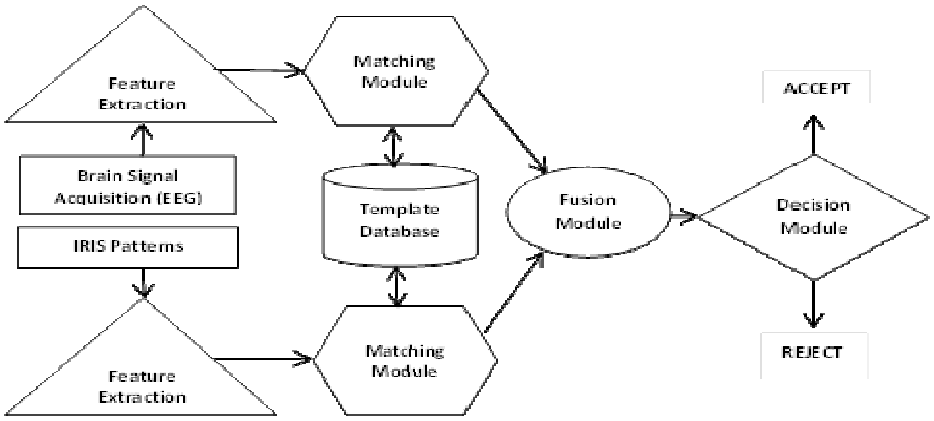


**FIGURE:1** Block Diagram for IRIS & Brain Forensics

## 3. METHODLOGY

### 3.1. IRIS Recognition System

Extraction of the IRIS image is more complicated. Since IRIS is small in size and dark in colour. The IRIS patterns are differentiated by several characteristics including ligaments, furrows, ridges, crypts, rings, corona, freckles, and a Zigzag collarette. Stability is one of the key advantages of IRIS recognition and it is suitable for one - many identification. Veri Eye Standard SDK (IRIS Extractor, IRIS Matcher, IRIS Client, IRIS server, IRIS BSS) used to extract IRIS Patterns in the Effective Manner.

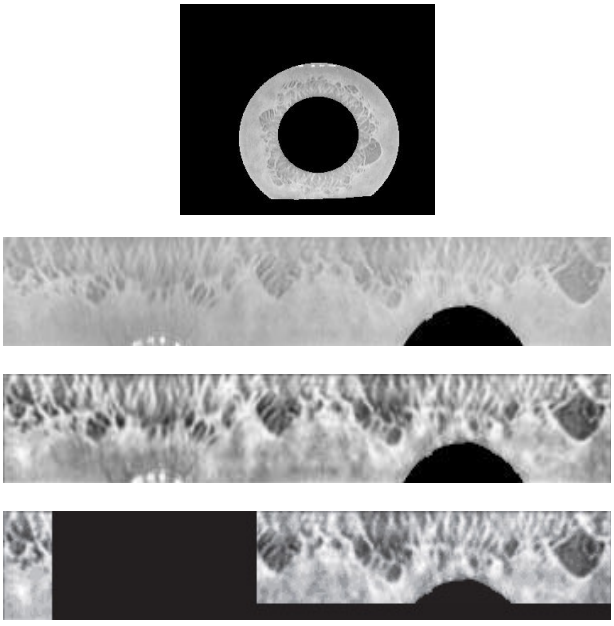

**FIGURE: 2** IRIS normalization (a) Segmented IRIS image
(b) Rectangular IRIS image (c) Enhanced IRIS image
(d) Region of interest in IRIS image

Extraction of the IRIS image is more complicated. Since IRIS is small in size and dark in colour. The IRIS patterns are differentiated by several characteristics including ligaments, furrows, ridges, crypts, rings, corona, freckles, and a Zigzag collarette. Stability is one of the key advantages of IRIS recognition and it is suitable for one - many identification.

Veri Eye Standard SDK (IRIS Extractor, IRIS Matcher, IRIS Client, IRIS server, IRIS BSS) used to extract IRIS Patterns in the Effective Manner.

IRIS Patterns not only contains exact information from the eye, but also several unwanted parts. (Ex. Eyelid, pupil etc). Under some conditions brightness may not be same and eye to camera distance may change the size of IRIS. To get an IRIS free of noise, independent on illumination and size, IRIS image pre-processing is done. For the purpose of analysis, the original image needs to be pre-processed to obtain a segmented and normalized image, then its texture is analysed and encoded to form an IRIS Feature vector. Finally, we compare templates to estimate similarity between Irises [7].

**3.2. Brain Wave Acquisition**

The human brain is the center of the human nervous system and it monitors and regulates the body's actions and reactions. It continuously receives sensory information, and rapidly analyses these data and then responds to the actions and functions. The electrodes used to measure electrical brain activity it is further amplified and stored on a memory device. The software presents the stimuli (Software for Data Acquisition), collects the EEG data, and analyses the data.

.

| *Type* | *Frequency* | *Use* |
|---|---|---|
| *Delta* | *<4 Hz* | *Occur during sleep, coma* |
| *Theta* | *4-7 Hz* | *Correlated with emotional stress* |
| *Alpha* | *8-12 Hz* | *Reduce amplitude with sensory stimulation or mental imagery* |
| *Beta* | *12-36 Hz* | *Can increase amplitude during intense mental activity* |
| *Mu* | *9-11 Hz* | *Diminishes with movement or intention of movement* |
| *Lambda* | *Sharp, Jagged* | *Correlated with visual attention* |
| *Vertex* | *-* | *Encephalopathy* |

**TABLE:1** Brain Waves signals and its Frequencies

EEG is usually by placing a number of electrodes to the scalp surface collected. There are several varieties commonly used electrodes silver tube electrodes, needle electrodes and adhesive electrodes, this system uses silver tube electrode in order to achieve the scalp with EEG measurement devices connection. Brain signal acquisition circuit includes EEG amplification, filtering, A / D conversion and USB interface circuit of four parts. It revealed by a specific pattern in the EEG (Electroencephalography).

This methodology tracks and records the Brain wave signals (EEG). Small metal discs with thin wires (electrodes) are placed on the scalp, and then send signals to a computer to track the Brain wave signals (EEG). Brain patterns forms different wave shapes that are commonly measured by 0.5 to 100 μV in amplitude. Usually EEG is 100 times lower than ECG signals. By means of Fourier transform power spectrum from the raw EEG signal is derived. In power spectrum contribution of sine waves with different frequencies are visible. Although the spectrum is

continuous, ranging from 0 Hz to one half of sampling frequency, the brain state of the individual may make certain frequencies more dominant.

Brain wave signals (EEG) also have some artifacts and EEG can carry many unwanted signals from brain. So the pre-processing is essential. For example [8]
• Interference from electronic equipment the 50 or 60Hz power supply signals,
• Electromyography (EMG) signals evoked by muscular activity,
• Ocular artifacts, due to eye movement or blinking.

Those unwanted components may bias the analysis of the EEG, and may lead to wrong conclusions. We have several modern techniques to reduce such artifacts, but each of those approaches has its own pros and cons. On a more fundamental level, however, it is clear that in order to reliably extract artifacts, one need to know how brain signals generally look like, and what information content they encode. Therefore, as our understanding of brain signals improves, it should become less difficult to detect and remove artifacts [8].

### 3.3. Feature Extraction

The IRIS Extractor, electrodes can read the IRIS patterns and Brain wave signals (EEG) respectively. Feature extraction should be defined with some invariant properties, Ability of discriminate pattern classes of interest, robust to noise, occlusion, Low measurement of cost and real time and lead to simple decision making strategies [9],[17]. In feature extraction image is classified by various algorithms and it will be visually recognized for unique patterns which is used for enrollment [10].
`

The experiment was conducted using data acquired in our labs for IRIS Patterns using Fuzzy Neural Network Algorithm can extract rules that yield much higher accuracy and robustness. Neural learning algorithm is applied for IRIS Classification, neural network especially for this task would be time consuming and selecting another wavelet would be more appropriate [12]. The IRIS recognition rate of Fuzzy Neural Network was 99.25%.

### 3.4. Matcher

The biometric matching system contains Pattern matching and the decision modules. The newly sensed biometric data will be first processed like the enrollment data, and the system will generate the pattern templates from the data. The pattern matching module compares the newly generated templates with those in the bio metric database and calculates match scores for final decision. If the matching score is higher than the predetermined threshold, the system identifies/verifies it.

In the matching module Binary coding scheme is used to obtain the feature vector into a binary code. Binary code-words converted into binary numbers. Boolean vectors or Binary numbers are always easier to compare and to manipulate in both IRIS and Brain. In order to code the feature vector we first observed some of its characteristics and all the vectors that we obtained have a maximum value that is greater than 0 and a minimum value that is less than 0.

If “Coefficient (Coef)” is the feature vector of an image than the following quantization scheme converts it to its equivalent code-word:

- If Coef (i) < 0 then Coef (i) = 0
- If Coef (i) >= 0 then Coef (i) = 1

The next stage is to compare two code-words to find out if they represent the same person or not [12].

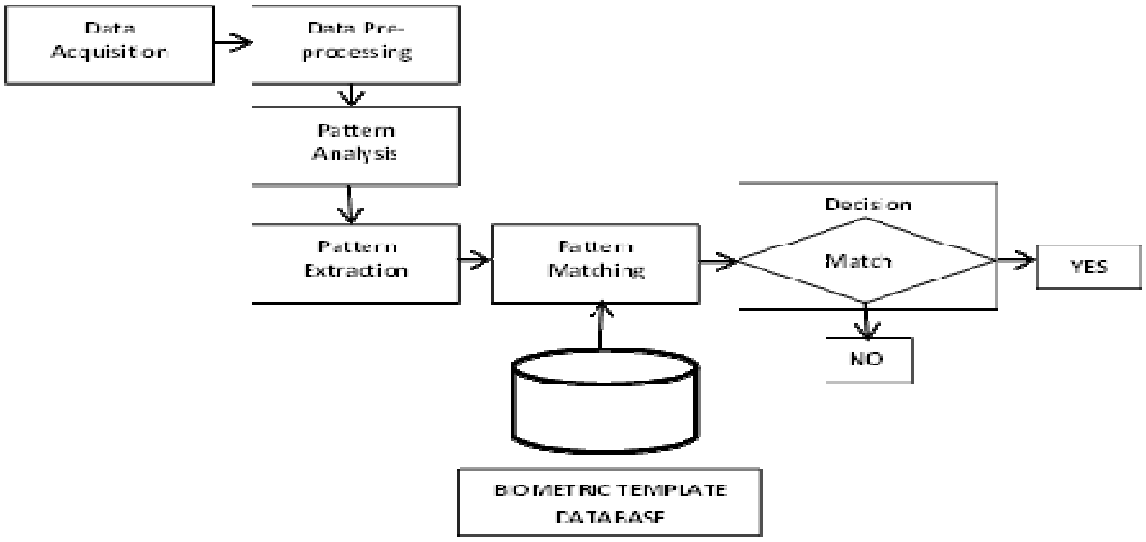


**FIGURE: 3** Matching Module

### 3.5. Template Database

The template that is created and stored is not the biometric data itself but instead the results from some kind of analysis and summary of the biometric data. These templates contain the unique characteristics of a user's biometric information, and they are the master copies that each future data acquisition would be compared to.

### 3.6. Matching Score Level Fusion

Matching score level fusion is one of the important biometric information fusion strategies, because matching scores are easily available and because they retain sufficient information to distinguish genuine matching from impostor matching. Multi biometric system divided into different subsystems each subsystem exploits one biometric trait to produce a matching score. Then these matching scores are normalized and integrated to obtain the final matching score is used for the final decision will give the authentication to the users [12]-[14].

## 4. RESULTS AND DISCUSSIONS

These methods can be triggered into different security levels such as secret services, military forces, police and criminal justice, especially in the frame of "homeland security", associated fears, concerns are that brain imaging may be used for "mind-reading" or reading the people's private thoughts and feelings, in the sense of polygraph, even without their consent and co-operation.

The nation's biggest threat is information piracy. The IRIS and brain biometrics can pave way to identify a sophisticated technical based solution to overcome information piracy. Airports, banks, military, commercial applications, enterprise-wide network security infrastructures, government IDs, secure electronic banking, investing and other financial transactions, and offices with documentation like passport, driving license, are required Highly secure identification and personal verification solutions. Thus Neuroimaging enrich the Digital Forensics Community with the help of Biometrics. IRIS and Brain recognition technology combines computer vision, the following results shows that IRIS, Brain wave signals (EEG) and its purpose is real time high confidence recognition.

| The Proposed Identification Method | IRIS | Brain Wave Signals(EEG) | Fusion |
|---|---|---|---|
| EER of the proposed method (%) | 3.21 | 4.16 | 2.12 |

**TABLE: 2** COMPARISON OF THE MATCHING PERFORMANCES

**5. CONCLUSION**

This paper will establish the digital forensics community and resolve the issues facing the digital forensics. IRIS and Brain has enormous features in biometrics to enhance diverse security levels and more secure than other biometric technologies. It helps to develop new tools, techniques, and methodologies in lie detection, crime detection and to detect the record of specific terrorist act or any incident stored in the brain and to intensify brain related methodologies in future. These ideas strongly suggest its future application in brain imaging studies.

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# Inhibition of Aldose Activity by Essential Phytochemicals of Cymbopogon Citratus (DC.) Stapf

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**Abstract**

The ambiguity of whether aldose reductase, an enzyme of polyol pathway, is linked to diabetes and its complication has been receded based on the recent studies made on the inhibition of its (Aldose reductase) activity. In our current study, we have used an *in silico* approach (molecular docking) to analyze the effect of essential phytochemicals obtained from *Cymbopogon citratus* on the aldose reductase activity. *C.citratus* is grown extensively in tropical countries including India for perfumery and pharmaceuticals. The essential phytochemicals of *C.citratus* like Myrcene, Citral, and Geraniol have been used as ligand for the molecular docking analysis with Aldose reductase as receptor. The docking analysis showed Myrcene, with binding energy of -8.76 Kcal/mol is best amongst Citral and Geraniol which are having binding energies of -7.24 Kcal/mol and -7.93 Kcal/mol respectively for inhibiting the activity of Aldose reductase.

**Keywords:** Aldose Reductase, Molecular Docking, Citral, Geraniol, Myrcene, Cymbopogon citratus

## 1. PRELIMINARIES

### 1. INTRODUCTION

From the past few decades the question of whether polyol pathway is responsible for diabetes retinopathy [2, 3, and 4] and other complications of human diabetes have been raised many times. Substantial amount of research on polyol pathway has revealed that the inhibition of aldose reductase activity [5] can lead to the cure of diabetic retinopathy. In this paper, we have presented an *in silico* analysis on the inhibition of aldose activity by the essential phytochemicals of *Cymbopogon citratus* [6]. Various species of *Cymbopogon* have been reported to control the hyperglycemia [7, 8] and other complication of diabetes. The essential phytochemicals were

extracted as stated in [1]. For the *in silico* analysis we have used Auto Dock [9] for the binding of ligand (essential phytochemicals of *C.citratus*) and receptor (Aldose reductase).

The hazardous polyol pathway of glucose metabolism becomes active when intracellular glucose levels are elevated [10, 14]. Aldose reductase (AR), the first and rate-limiting enzyme in this pathway, reduces glucose to sorbitol using NADPH as a co-factor; sorbitol is then metabolized to fructose by sorbitol dehydrogenase that uses NAD+ as a cofactor. The polyol pathway leads to several damaging effects. Sorbitol being an alcohol, is polyhydroxylated, and strongly hydrophilic, does not diffuse readily through cell membranes and accumulates intracellularly with possible osmotic consequences [10]. The fructose produced by the polyol pathway can become phosphorylated to fructose-3-phosphate [15, 16], which is broken down to 3-deoxyglucosone; both compounds are powerful glycosylating agents that enter in the formation of advanced glycation end products (AGEs) [15]. The usage of NADPH by AR may result in fewer co-factors available for glutathione reductase, which is critical for the maintenance of the intracellular pool of reduced glutathione (GSH). This would lessen the capability of cells to respond to oxidative stress [17]. Compensatory increased activity of the glucose monophosphate shunt, the principal supplier of cellular NADPH, may occur [17]. The usage of NAD by sorbitol dehydrogenase leads to an increased ratio of NADH/NAD+, which has been termed as "pseudohypoxia" and linked to a multitude of metabolic and signaling changes known to alter cell function [18]. It has been proposed that the excess NADH may become a substrate for NADH oxidase, and this would be a mechanism for generation of intracellular oxidant species [19]. Thus, activation of the polyol pathway, by altering intracellular tonicity, generating AGEs precursors, and exposing cells to oxidative stress perhaps through decreased antioxidant defenses and generation of oxidant species, can initiate and multiply several mechanisms of cellular damage.

Retinal ganglion cells, Muller glia, and vascular pericytes and endothelial cells are endowed with aldose reductase in all species studied, including humans [20]. Hence, these cell types are exposed to polyol pathway activation in diabetes. These are also the cells that manifest the best-known changes or damage in diabetes [21]. The biochemical consequences of polyol pathway activation have been studied in the whole retina of diabetic animals. The best-documented are the accumulation of sorbitol and fructose [22, 23], and the generation or enhancement of oxidative stress. Insofar as indices of polyol pathway-induced oxidative stress are measurable in preparations of the whole retina, the abnormalities are likely to occur in most cell types or at least in cells that are highly represented in the whole retina. Muller glia cells are the candidates because they are large cells present in high number in the retina [24].

### 1.1. Cymbopogon Citratus

*Cymbopogon citratus* (DC.) Stapf. (West Indian lemongrass or citron grass), *C.flexuosus* (steud) Wats. (East Indian lemongrass or Cochin lemongrass) and *C.pendulus* (nees) Wats (North Indian lemongrass) [1, 6]. They are extensively cultivated besides their wild status in South and Central America and many other tropical countries including India for perfumery and pharmaceuticals. *C.citratus* is well known to produce essential oils up to 1.5 %( dry weight) with characteristic 'lemon aroma' dominated by Citral, which is a mixture of isomeric, acyclic, monoterpene aldehydes (Guenther, 1950; Weiss, 1997). According to the reports, lemon grass oil consists of 75-85% Citral, which is natural geranial (Trans – Citral, Citral -A) and 40% neral (Citral, Citral-B), Geraniol (aromatic alcohol), and Myrcene (characteristic in C.citratus) (Formacek and Kubeezka, 1982). Citral is used as a raw material largely in perfumery, cosmetics and pharmaceutical industries.

Earlier studies made by the author on *C.citratus* [1] was focused on the generation of *in vitro* variants (long and short morphotypes) using young leaf segments. Further, the essential oils were extracted; GC analysis were made on long and short morphotypes and compared with controlled plants.

### 1.2. Auto Dock

The field of molecular docking and computer- assisted drug design from the last few decades has started to be a most important field. Now one can find a few programs that work with various accuracy and features, e.g. Auto Dock [9], DOCK [25], and Sybyl's [26]. A common feature in these programs is that they simulate or match, and in this way try to optimize the binding conformation between the two molecules. They use different techniques to accomplish this, e.g. simulated annealing [27], genetic algorithms [28], flexible molecular bonds, rigid bodies, spheres and grid boxes. In the present work we have used Auto Dock exclusively along with one of its search method called Lamarckian genetic algorithm (LGA) [29]. The macromolecule is rigid and fixed while the ligand is flexible and can both translate and rotate. Auto Dock uses a rapid grid-based method for finding the lowest binding energy of the bound conformation. These grids are calculated in advanced (i.e. before the actual docking) and one for each atom type present. The size of the grid box can be set manually and placed at a certain position. These boxes create maps over the molecules that are used during the docking, to exclude atoms of no interest and also to speed up the docking calculations.

## 2. PRELIMINARIES

### 2.1 Methodology

For the molecular interaction between the essential phytochemicals obtained from *C. citratus* [1] and the enzyme Aldose Reductase [30], we have used Auto Dock. Although, Autodock uses a wide range of algorithm like simulation annealing , genetic algorithm , Lamarckian algorithm etc, but, for the biomolecular interaction analysis between the receptor (Aldose) and ligand (phytochemicals obtained from *C. Citratus*) we have used Autodock's Hybrid Lamarckian Genetic Algorithm LGA [29]. Hybrid Lamarckian Genetic Algorithm utilizes Lamarckian notation that is an adaptation of an individual to its environment which can be inherited by its offspring. Prior to the docking analysis by using autodock, the ligand and the receptor molecule should be modeled in such a way that they contain the entire parameter and set of values, which are required by LGA while docking. The autodock experiment usually divides the ligand and the receptor into five different input files.

- A pdbqt [31] file for ligand that encodes the torsion tree
- A pdbqt file for receptor
- A Grid Parameter File(GPF) for the autogrid calculation
- A Docking Parameter File (DPF) for autodock calculation
- A pdbqt file containing the flexible residues

Both receptor and the ligand can be modeled into the above mentioned files in the following way

#### 2.1.1 Preparing the Receptor file

Aldose reductase which we have taken as our receptor molecule for the docking analysis with the essential phytochemicals of *C.citratus* was obtained from the Brook haven protein data bank [32] with resolution of 1.65A°. The PDB file [1ADS] was first edited by adding all the hydrogen bonds to it. The catalytic site of 1ADS consists of residues such as Asp, Tyr, Lys and His. The gaister charges are then added to the protein molecule and saved as PDBQT macro molecule. The Aldose along with Hydrogen bonds is as shown in Fig 1.

#### 2.1.2 Preparing the Ligand file

Based on the purpose of the study, the essential phytochemicals obtained from *C. citratus* [1], such as Myrcene, Citral and Geraniol were considered as ligand molecules. The ligand files were prepared using Chemsketch [33]. The ligand files are then converted into PDB file format by adding all the hydrogen bonds to it using Bable. Adding hydrogen bonds is necessary for the uniform gaister charge distribution which is required during docking. In a docking procedure either ligand or receptor molecule can set free to rotate. The free rotation of either ligand or receptor

**FIGURE 1:** Aldose with Hydrogen Bonds

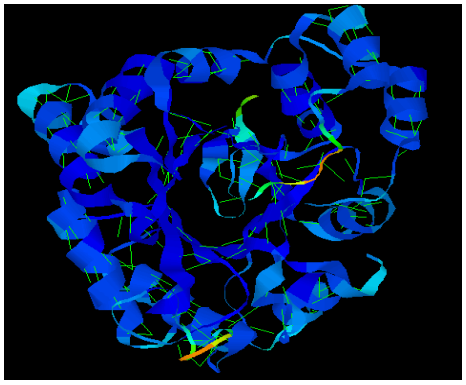
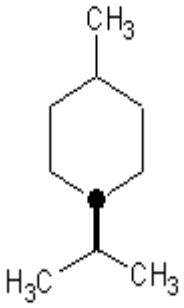


**FIGURE 2:** 7-methyl-3-methylene-1,6-octadiene(m)




provides the best execution of LGA in which one species is kept rigid and other allow rotating freely. In our analysis we have set the receptor molecule (Aldose) as rigid species and ligand species is set free to rotate around it. The torsion tree root (around which the ligand rotates) is then detected for all the three ligands. For Citral the torsion root is detected at carbon atom C6 where torsion root is represented by a black dot and allowable rotational bonds with dark black lines as shown in [Fig 3].

**FIGURE 3:** 3, 7-dimethyl-2, 6-octadienal (c) (g)

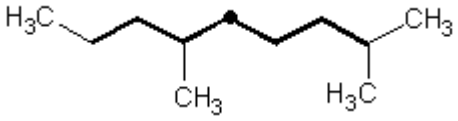
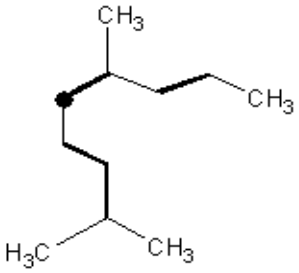



**FIGURE 4:** 3, 7-dimethyl-2, 6-octadien-l-ol




For Myrcene the torsion root detected at carbon atom C6 where the modified Myrcene with torsion root represented by a dot and one allowable rotational bond by black line as shown in [Fig 2]. The modified Geraniol is as shown in [Fig 4] with torsion root represented by a black dot and four allowable rotational bonds with dark black lines.

### 2.1.3 Preparing the Grid Parameter File

A grid is a system space under consideration. Grid is 3D space in which the receptor [1ADS] is embedded and a probe atom is placed at each grid point. An affinity is calculated for each type of atom in a substrate, mainly carbon, oxygen, nitrogen and hydrogen as well as grid of electrostatic potential either using a point charge of +1 as probe, or using Poisson – Boltzmann finite difference method such as DELPHI. Auto dock requires a pre calculated grid maps, one for each atom type present in the ligand. A grid map consist of 3D lattice of regularly spaced point, surrounding (either entirely or partially) the region of interest in the macromolecule. The grid size is selected such that it covers the entire molecule to provide extreme freedom of rotation to the ligand molecule.

## 2.2 Results and Discussion

Based upon the limited data and some earlier findings on Aldose reductase inhibitors obtained from natural sources such as flavonoids, coumarins, stilbenes, monoterpenes, and related aromatic compounds, it has been well acknowledged that plant derived extracts and phytochemicals are potential alternatives to synthetic inhibitors against Aldose reductase [33-37], although *in vivo* efficacy and clinical utility remain to be evaluated. In order to explore the inhibitory mechanism of natural compounds/phytochemicals towards Aldose reductase, bioinformatics plays a major role, where docking can be done using computer software to find out the binding sites and docking mechanisms. This provides a clear view on how the drug acts upon Aldose reductase and inhibits its activity. The results imply that methods designed to normalize Aldose reductase activity could be of significant benefit in the prevention and treatment of diabetic retinopathy [38]. From the docking results obtained, it can be concluded that the phytochemicals effectively docked into the binding site of Aldose reductase protein indicating that they are efficient drug compounds. The docking of Aldose reductase by myrcene showed best binding energy as compared to other two compounds viz., citral, geraniol. All the three components have more or less similar docking binding energies and so it might be expected that all the three active components can be used for synergistic inhibition on Aldose reductase activity under *in vivo* condition. These results suggest that active components from *C. citratus* would have some pharmacological actions against Diabetes mellitus. Further this may be confirmed by drug trials in animal models to find out the optimum dose and its efficiency in inhibiting Aldose reductase activity and reduce diabetic related complications.

In view of the above, it was felt that molecular docking of Aldose reductase activity inhibition by using the essential phytochemicals of *C. citratus* such as myrcene, citral and geraniol would be helpful to understand the underlying mechanism. This work would provide a clear understanding on the mode of action of the above mentioned plant components of *C. citratus* individually or synergistically against Aldose reductase and can be used as an inhibitory drug to reduce diabetic related complications. Based on the previous analysis made on variation in contents of essential oil *in vivo* and *in vitro* plants of *C. citratus* [1] we have concluded the percentage of essential oils viz Citral, Myrcene and Geraniol as shown in table- 2 which shows the % variation in concentration of essential oils in *in vivo* and *in vitro* (both long and short morphotypes) plants. Since Myrcene is most effective for Aldose activity inhibition, as concluded from Auto Dock results, obtaining Myrcene from *in vivo* plants is most efficient than obtaining it from *in vitro* plants for the inhibition of aldose reductase activity.

In order to run Auto dock, grid maps have to be calculated. The dimension of grid points in x y z, directions were fixed as 90, 90, 90 respectively, this covers the active site extensively and allows the ligand move without any constraint regarding the box size. Spacing between grid points was kept as 0.375 Å with a common grid center. In the docking of three ligands viz: Citral, Geraniol and Myrcene, three docking parameter files (DPF) were generated one for each ligand by a Python script that use the methods in Auto Dock. The script takes one pdbqs file, loops over the pdbq file and sets the name of the maps and the ligand in the parameter file. It also sets the Lamarckian Genetic Algorithm (LGA) to be used with a population size of 50 individuals. These 50 were calculated at 10 different runs (i.e. 10 dockings) and the runs had two stop criteria-

- A maximum of 1000330 energy evaluations.
- A maximum of 993 generations.

The ligands were set to start in a random position and conformation, the translations were set to have a maximum of 2 Å/step and the torsion, both had a maximum at 50°/step. The elitism number was set to 1. The mutation rate and the crossover rate were 0.02 and 0.80 respectively. The probability that an individual in the population will undergo a local search was set to 0.06 and the constraint used in the Pseudo-Solis and Wet's local search was set to a maximum of 300 iterations per search. The size of the local search space was 1.0 and the smallest step that the

local search could take before the ending was set to 0.01. This creates a docking parameter file for each docking in the directory.

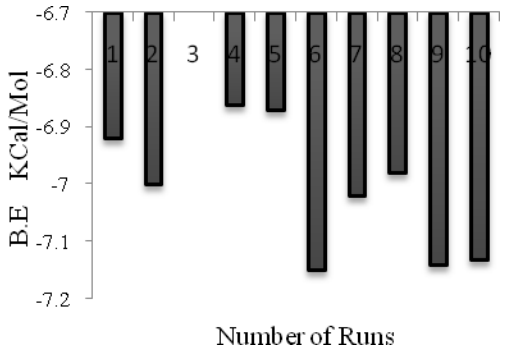
Docking results obtained showed the binding energy of all the three ligands (Citral, Geraniol and Myrcene) to the receptor molecule Aldose. Table 1 shows the binding energies of all the three ligands with receptor Aldose and it can be seen that Myrcene has the best binding energy whereas Citral and Geraniol are not much reliable for binding to receptor molecule with almost same binding energies.

**TABLE 1:** Binding energy and Mean Binding Energy

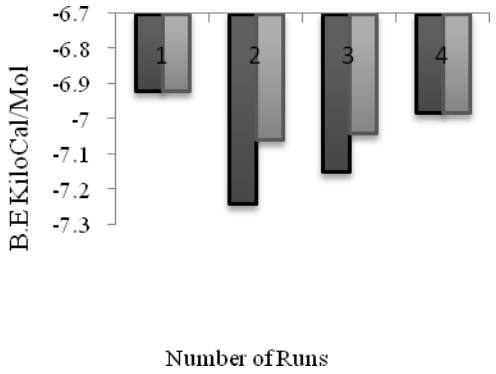
| **Ligand** | **Binding Energy Kilo Cal/Mol** | **Mean Binding Energy Kilo Cal/Mol** |
|---|---|---|
| Geraniol | -7.93 | -7.90 |
| Citral | -7.24 | -7.06 |
| Myrcene | -8.76 | -8.75 |

Based on the algorithm used, the docking result also showed, the Root Mean Square Deviations (RMSD) and Clustering data. Both, RMSD and clustering data is obtained based on the binding energy with respect to number of runs in which docking took place. Graph 1 shows the RMSD data of Citral and it can be seen that the binding energy of Citral varies in the range of -6.9 Kilo Cal/Mol to -7.1 Kilo Cal/Mol. Graph 2 shows the clustering of Citral with receptor ADS, wherein the Citral shows the best four clustering out of total 10 dockings. Both the lowest and mean binding energy of Citral clustering varies between -6.92 Kilo Cal/Mol to -6.98 Kilo Cal/Mol, with best lowest binding energy of -7.24 Kilo Cal/Mol and best mean binding energy of -7.06 Kilo Cal/Mol

**Graph. 1-** Citral RMSD

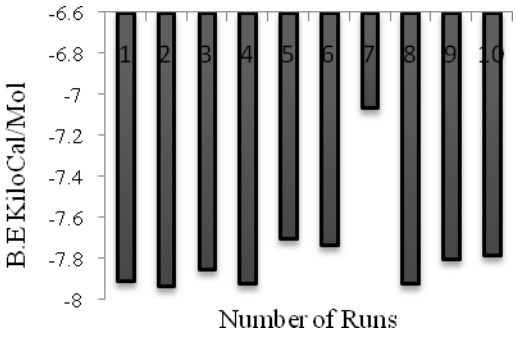



**Graph. 2-** Citral Clustering

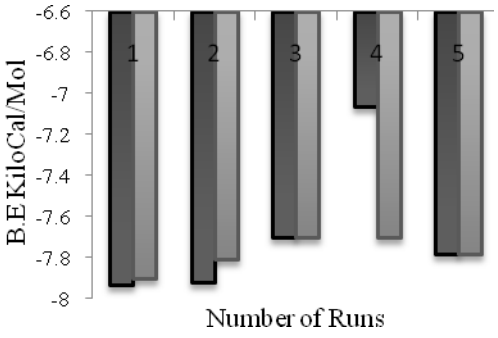



The RMSD and Clustering data of Geraniol is also generated as shown in Graph 3 and Graph 4 respectively. The binding energies in RMSD analysis of Geraniol [Graph 3] was found to be almost constant with respect to all the number of runs, varying in the range between -7.9 Kilo Cal/Mol to -7.7 Kilo Cal/Mol in all the 10 runs (10 Dockings). The clustering of Geraniol [Graph 4] shows the five best clustering out of total 10 runs with best lowest binding energy of -7.93 Kilo Cal/Mol and the best mean binding energy -7.9 Kilo Cal/Mol.

**Graph. 3-** Geraniol RMSD



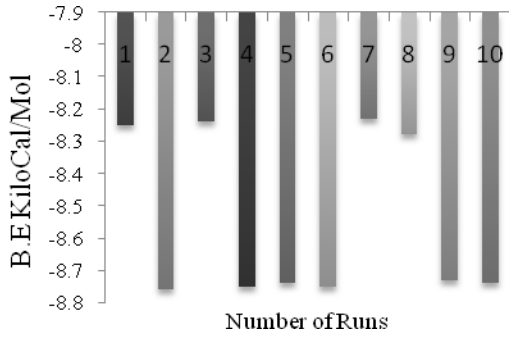

**Graph. 4-** Geraniol Clustering



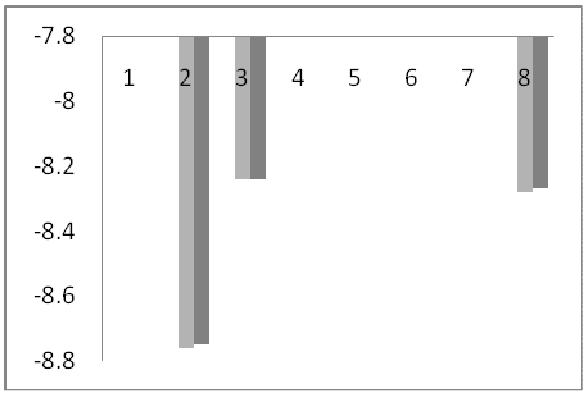

Similarly, the RMSD and clustering data of Myrcene is obtained as shown in [Graph 6] and [Graph 7]. Myrcene, in fact, showed the best binding energies both in RMSD as well as clustering

analysis. In RMSD analysis [Graph 6] the binding energy of Myrcene varies between the range of -8.2 Kilo Cal/Mol to -8.7 Kilo Cal/Mol in total of 10 runs (10 Dockings). The clustering of Myrcene [Graph 7] showed best three clustering out of total 10 with best lowest binding energy of -8.76 Kilo Cal/Mol and best mean binding energy of -8.75 Kilo Cal/Mol.

**Graph. 5-** Myrcene RMSD




**Graph. 6-** Myrcene Clustering




From the docking results obtained, it can be concluded that the compound Myrcene shows the best binding energy as compared to other two compounds (Citral and Geraniol) of *C. citratus* with respect to receptor Aldose. Based on the previous analysis made on variation in contents of essential oil *in vivo* and *in vitro* plants of *C.citratus* [1] we have concluded the percentage of essential oils viz Citral, Myrcene and Geraniol as shown in table- 2.

**TABLE 2:** Composition of Essential Oils of *C.citratus*

| RI | Compound | Natural (%) | Long morphotype | Short morphotype |
|---|---|---|---|---|
| 985 | Myrcene | 45.22 | -- | 14.55 |
| 1242 | Geraniol | 1.59 | 1.67 | 2.18 |
| 1252 | Citral | 44.33 | 49.41 | 43.36 |

Table- 2 shows the % variation in concentration of essential oils in *in vivo* and *in vitro* (both long and short morphotypes) plants [1a]. Since Myrcene is of most important for Aldose activity inhibition, as concluded from Auto Dock results, obtaining Myrcene from *in vivo* plants is most efficient than obtaining it from *in vitro* plants, both long and short morphotypes for the inhibition of aldose reductase activity.

### 2.3 Conclusion

Overall the obtained data highlight the importance of phtytochemical from *Cymbopogon citratus* on the aldose reductase activity which will reduce diabetic complications for or great number of diabetes patient. It is in accordance with previously reported on the aldose redutase inhibitory activities of a number of phytochemicals.

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