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INSILICO COMARATIVE MODELING OF MATURASE K PROTEIN IN *CYMBOPOGON MARTINI* PLANT

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ABSTRACT

In recent years, due to environmental, health and safety concerns, there has been an increasing interest in replacing synthetic compounds with natural products. Essential oils of aromatic plants are of great interest among natural products because of their relatively low or negligible toxicity and high volatility and biodegradability. In recent years, due to environmental, health and safety concerns, there has been an increasing interest in replacing synthetic compounds with natural products. Cymbopogon martini (Gramineae) is a medicinal and aromatic plant of great importance and rich in essential oils. Essential Palmarosa-derived oils have shown exceptionally good antimicrobial, antifungal, antiviral, antihelmintic, antioxidant and cytotoxic characteristics. Maturase k is one of the antimicrobial proteins found in Cymbopogon martini. The main objective of this article is to cover the various Maturase k protein insilico analyzes.

KEYWORDS: Cymbopogon martini, Palmarosa, essential oil, Maturase k protein, medicinal and aromatic plants, chemical compound.

INTRODUCTION

Cymbopogon martinii is a grass species in the genus Cymbopogon (Lemongrasses) native to India and Indochina but widely grown for its aromatic oil in many places. The common name palmarosa (palm rose) is best known because it smells sweet and rose like.[1] Cymbopogon martinii is an extremely important member of the Gramineae family, well known for its high oil content. Essential oils (volatile oils, ethereal oils, aetherolea) are hydrophobic concentrated fluids containing plant volatile aromatic compounds. Oil is "essential" in that it

contains the "essence" of the extract of the plant, the characteristic fragrance of the plant from which it originates.[2] Plants synthesize many types of secondary metabolites or specialized phytochemicals, an important group of which are essential oils (EOs). These compounds can be extracted by various procedures (e.g. hydrodistillation and steam distillation) from plant tissue (e.g. stem, leaves, flowers and roots). Terpenes, alkaloids (N-containing compounds) and phenolics constitute the largest groups of secondary metabolites.[3] [4] The shikimic acid pathway is the basis of the phenolic biosynthesis, while the terpenes consisting of isoprene units originate from the mevalonate pathway. Essential oils mainly contain terpenes, which are commonly used in pharmaceutical industries and have therapeutic advantages and promote welfare, especially when it used in aromatherapy Procedures.[5] Cymbopogon martini's essential oils are rich in monoterpenes. Essential oils and their components of Cymbopogon species are known for their antihelmintic, antiparasitic, anti - inflammatory, anticonsulvant and antioxidant activities.[6,7] The presence of citral (a mixture of geranial and neral), geraniol, citronellol, citronella, linalool, elemol, 1,8-cineole, limonene, geraniol, β-caryophyllene, methyl heptenone, geranyl acetate and geranyl formats in the essential oils of Cymbopogon martini has been shown in several previously published reports. In addition, genetic, environmental and geographical conditions greatly influence the composition of the essential oil components. The essential oils of Cymbopogon martini are biosynthesized in the fast - growing leaves and stored in parenchymal tissue in specific oil cells.[8]

Pharmacological Activities

C's essential oils. Martinii were studied and showed high anthelmintic activity against Caenorhabditis elegans with a value of ED50 of 125.4 µg / Ml.[9] This was caused mainly by geraniol (a major chemical component). Palmarosa oil has also shown anthelmintic activity against the Pheretima posthumous Indian earthworm, causing paralysis and death in a short time.[10] Essential oil martinii (palmarosa) is used as fumigation to control beets such as Callosobruchus chenesis and Tribolium castaneum growing in stored grain. Palmarosa oil is used in medicine as a remedy for lumbago, stiff articulations and skin diseases. Oil C. Oil of C. Martinii leaves obtained by distillation were given orally to study their effect on the exudative phase of inflammatory reactions using the paw oedema technique induced by Carrageenan.[11] Oil C. Oil of C. Martini showed dose-dependent anti - inflammatory activity comparable to diclofenac sodium Palmarosa showed significant positive effects on several pathologies of the central nervous system, mainly neuralgia, epilepsy and anorexia. Some reports about its effects;. Because of its antimicrobial, antigenotoxic and antioxidant

activities, martinii has attracted the attention of many researchers. Geraniol, C's major component. Martinii EO is an abundant acyclic monoterpenoid in many plants. It can represent a new class of pancreatic and colon cancer therapeutic agents and has several biological properties, including antimicrobial, antioxidant and anti – inflammatory activities.[12] Sinha et al. investigated the possible antigenotoxic and antioxidant properties of palmarosa and citronella essential oils in human lymphocytic cells.[13] Two spectrophotometric methods revealed the antioxidant activity of the essential oils; DPPH + free radical scavenging and lipid peroxidation tests. Palmarosa and Citronella oil showed a high level of anti-radical activity with higher activity in Palmarosa.[14] Palmarosa and Citronella oils have IC50 values of 187,503 and 215,763 µg / ml respectively. The IC50 value is inversely related to the test sample scavenging activity. Egg yolk lipids are rapidly peroxidized without enzymes in the presence of ferrous sulphate.[15] Palmarosa and Citronella oils concentration-dependent inhibited lipid peroxidation with IC50 values of 198.109 and 206.286 µg / ml respectively. Ascorbic acid (100 µM) inhibition of lipid peroxidation was about twice as high as essential oils. The antigenotoxic effect on human lymphocyte cells (cell viability measurement, DNA damage) was investigated using the tripan blue dye exclusion test, plasmid pBR322 DNA strand scission test and comet test. The essential oils showed good methyl methane sulphonate (MMS) and hydrogen peroxide antigenotoxic activity.[16] Aromatherapy is a traditional treatment in which the aromatic molecule of essential oils passes through the nasal cavity and adheres to the olfactory epithelium and directly stimulates the hippocampus and limbic amygdaloidal body.[17] This stimulates the control of the autonomic nervous system and internal secretory control by changing a number of vital reactions.[18] The inhalation of aromatic compounds in essential oils is the reason for the name ' aromatherapy,' and this therapy can sedate or stimulate the individual. Literature reports describe the benefits of the use of essential oils in aromatherapy for the well - being of individuals, including improvements in mood, stress, anxiety, depression and chronic pain.[19] The inhalation of essential oils increased blood pressure and renal sympathy, which reinforces the idea that these components interact with the central nervous system and cross the blood - brain barrier. The highly lipophilic volatile organic compounds can easily cross the blood - brain barrier and exert their neuro pharmacological effects.[20]

METHODOLOGY

Sequence Retrieval system

The Maturase k protein sequence was retrieved from NCBI in order to perform Primary and

secondary structure prediction.[21]

Primary and Secondary analysis

The retrieved gene Maturase k coded protein sequences was applied into Protparam and Gor server in order to predict the Primary and secondary structures of the protein sequences.

Protein modeling

The retrieved gene Maturase k coded protein sequences was applied into Swiss model server[22] in order to predict the 3 Dimensional structures of the protein sequences.

Protein Structure Visualization

The modelled protein 3D structure was viewed with the help of advanced molecular visualization software called Discovery Studio in order to identify the structural regions and to classify the entire 3D structure elements.[23]

RESULTS AND DISCUSSION

Sequence Retrieval system Ncbi

>AMA19923.1 maturase K, [Cymbopogon martinii]

SLIQVEIQMEKFEGYSEKQKSRQHYFVYPLLFQEYIYAFAHDYGLNGSEPVEICGCNN
KKFSSILVKRLI
IRMYQQNFLINSVNYPNQDRLFDHCNYFYSDFYSQILSEGFAIVVEIPLSLGQLSCPEE
KEIPKFQNLQS
IHSIFPFLEDKFLHLHYLSHIEIPYPIHLEILVQLLEYRIQDVPSLHLLRFFLHYYSNWNS
LITSMKSIF
LFSKENKRLFRFLYNSYVSEYEFFLLFFRKQSSCLRLTSSGTFLERIIFSGKMEHFGVM
YPGFLRKTIWF
FMDPLMHYV

The above results shows the fasta format sequence of Maturase k protein

Primary analysis

ProtParam

User-provided sequence

10 20 30 40 50 60
SLIQVEIQME KFEGYSEKQK SRQHYFVYPL LFQEYIYAFA HDYGLNGSEP VEICGCNNKK

70 80 90 100 110 120
FSSILVKRLI IRMYQQNFLI NSVNYPNQDR LFDHCNYFYS DFYSQILSEG FAIVVEIPLS

130 140 150 160 170 180
LGQLSCPEEK EIPKFQNLQS IHSIFPFLED KFLHLHYLSH IEIPYPIHLE ILVQLLEYRI

190 200 210 220 230 240
QDVPSLHLLR FFLHYYSNWN SLITSMKSIF LFSKENKRLF RFLYNSYVSE YEFFLLFFRK

250 260 270 280
QSSCLRLTSS GTFLERIIFS GKMEHFGVMY PGFLRKTIWF FMDPLMHYV

Number of amino acids: 289

Molecular weight: 34802.31

Theoretical pI: 6.85

Amino acid composition: CSV format

Ala (A) 3	1.0%
Arg (R) 12	4.2%
Asn (N) 13	4.5%
Asp (D) 7	2.4%
Cys (C) 5	1.7%
Gln (Q) 15	5.2%
Glu (E) 21	7.3%
Gly (G) 10	3.5%
His (H) 12	4.2%
Ile (I) 24	8.3%
Leu (L) 36	12.5%
Lys (K) 15	5.2%

Met (M)	7	2.4%
Phe (F)	30	10.4%
Pro (P)	12	4.2%
Ser (S)	28	9.7%
Thr (T)	4	1.4%
Trp (W)	2	0.7%
Tyr (Y)	21	7.3%
Val (V)	12	4.2%
Pyl (O)	0	0.0%
Sec (U)	0	0.0%
(B)	0	0.0%
(Z)	0	0.0%
(X)	0	0.0%

Total number of negatively charged residues (Asp + Glu): 28

Total number of positively charged residues (Arg + Lys): 27

Atomic composition

Carbon C	1634
Hydrogen H	2422
Nitrogen N	394
Oxygen O	427
Sulfur S	12

Formula: $C_{1634}H_{2422}N_{394}O_{427}S_{12}$

Total number of atoms: 4889

Extinction coefficients

Extinction coefficients are in units of M^{-1} cm^{-1}, at 280 nm measured in water.
Ext. coefficient 42540
Abs 0.1% (=1 g/l) 1.222, assuming all pairs of Cys residues form cystines
Ext. coefficient 42290
Abs 0.1% (=1 g/l) 1.215, assuming all Cys residues are reduced

Estimated half-life

The N-terminal of the sequence considered is S (Ser).

The estimated half-life is: 1.9 hours (mammalian reticulocytes, in vitro).

>20 hours (yeast, in vivo).

>10 hours (Escherichia coli, in vivo).

Instability index

The instability index (II) is computed to be 61.57

This classifies the protein as unstable.

Aliphatic index: 94.05

Grand average of hydropathicity (GRAVY): -0.048

The above results shows the primary sequence analysis of Maturase k protein.

Secondary analysis

GOR4 result for : UNK_535920

Abstract GOR secondary structure prediction method version IV, J. Garnier, J.-F. Gibrat, B. Robson, Methods in Enzymology,R.F. Doolittle Ed., vol 266, 540-553, (1996)

View GOR4 in: [AnTheProt (PC) , Download...] [HELP]

10 20 30 40 50 60 70

| | | | | | |

SLIQVEIQMEKFEGYSEKQKSRQHYFVYPLLFQEYIYAFAHDYGLNGSEPVEICGCNN

KKFSSILVKRLI

ccccccchhhhhcchhhccccceeeechhhhhhhhhhhcccccccccceeeeeccccccchhhhhhhh

IRMYQQNFLINSVNYPNQDRLFDHCNYFYSDFYSQILSEGFAIVVEIPLSLGQLSCPEE

KEIPKFQNLQS

hhhhhhceeeccccccccccceeccccccccccchhhhhhcceeeeeccccccccccccccccccccc

IHSIFPFLEDKFLHLHYLSHIEIPYPIHLEILVQLLEYRIQDVPSLHLLRFFLHYYSNWNS

LITSMKSIF

ccccccccchhhhhhhcccccccccchhhhhhhhhhhcccccchhhhhheeeceeccceeeeechhhhh

LFSKENKRLFRFLYNSYVSEYEFFLLFFRKQSSCLRLTSSGTFLERIIFSGKMEHFGVM

YPGFLRKTIWF

hhhhhhhhhheeeccccchhhhhhhhhcccccceeeccccccceeeeeeccccccceeececccceeeeee

FMDPLMHYV

eecceeeec

Sequence length : 289

GOR4 :

Alpha helix (Hh) : 87 is 30.10%

3_{10} helix (Gg) : 0 is 0.00%

Pi helix (Ii) : 0 is 0.00%

Beta bridge (Bb) : 0 is 0.00%

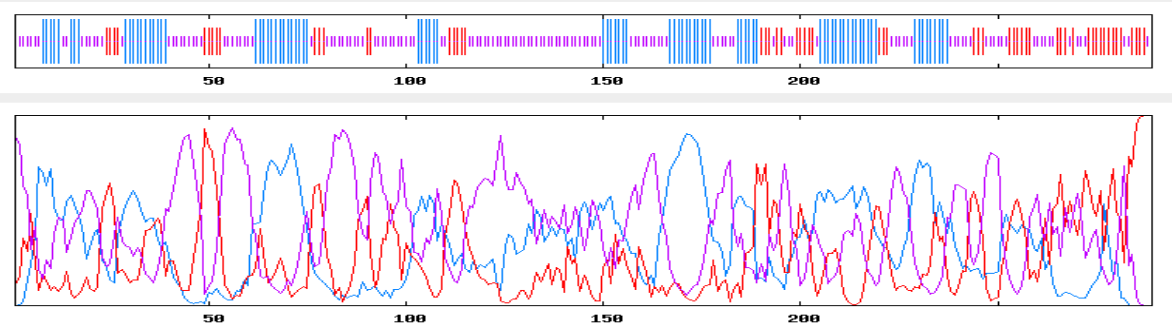
Extended strand (Ee) : 58 is 20.07%

Beta turn (Tt) : 0 is 0.00%

Bend region (Ss) : 0 is 0.00%

Random coil (Cc) : 144 is 49.83%

Ambiguous states (?) : 0 is 0.00%

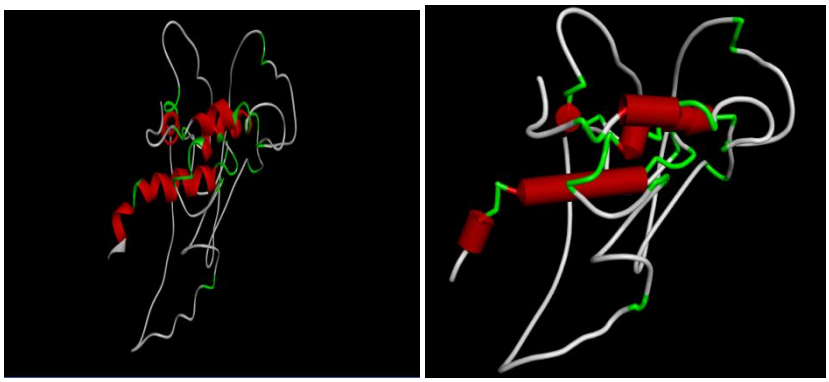


Other states : 0 is 0.00%

The above results shows the secondary sequence analysis of Maturase k protein.

Protein modeling

Swiss Model



Hydrophobic yellow1 ala, val, phe, pro, met, ile, leu polar pink ser, thr, tyr, his, cys, cyss, asn, gln, trp, gly charged (+) blue lys, arg charged(-) red asp, glu.

CONCLUSION

Cymbopogon martinii is an extremely important member of the Gramineae family, well known for its high oil content. Essential oils (volatile oils, ethereal oils, aetherolea) are hydrophobic concentrated fluids containing plant volatile aromatic compounds. Oil is

"essential" in that it contains the "essence" of the extract of the plant, the characteristic fragrance of the plant from which it originates.[24] Various compounds have been isolated and identified from Cymbopogon martini essential oil. Comparative ("homology") modeling approximates the 3D structure of a target protein for which only the sequence is available, provided an empirical 3D "template" structure is available with >30% sequence identity.[25] Homology modeling can produce high - quality structural models when the target and the template are closely related, which has inspired the formation of a consortium of structural genomics dedicated to the production of representative experimental structures for all classes of protein folds.[26] We have predicted the structure based on the sequence in the maturase k protein (cymbopogon martini). A comprehensive protein study can also be used in research.

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