Bioinformatics Approach For Conservation Of Fauna and Flora Through Bioprospecting

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Citation

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Abstract

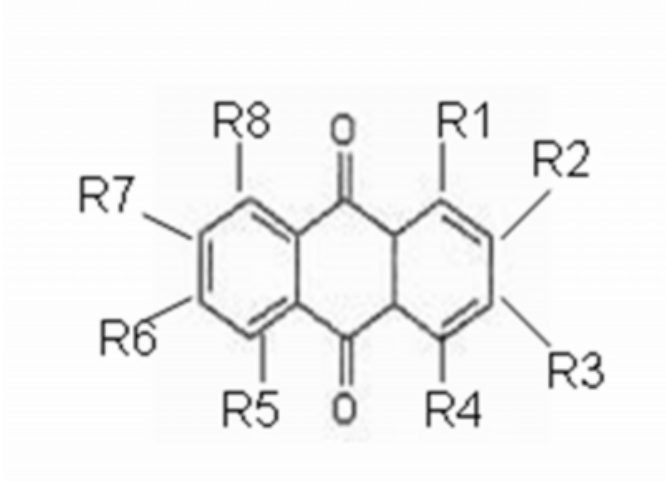
Varieties of valuable compounds like- cosmetics are extracted from various animals. Many companies have catered to this expanding market of cosmetics by introducing various makeup types for which they use vibrant colors that are derived from some unexpected sources, ranging from crusted insects to rust, which is responsible for diminution of biodiversity. Therefore there is a strong need to look for alternative source for these compounds (Bioprospecting). In this paper, a bioinformatics approach has been used to analyze the molecular evolution of known valuable compounds like anthraquinone by analysis of pathway and construction of phylogenetic trees. Phylogenetic analysis provides new horizons for this type of study and shows their worthwhile by giving the answers of their origin, development and other characteristics. The phylogenetic analysis of enzymes was incorporated to know, which species are related and which one is the ancestral species. Bioinformatics database, tools and software which were used in the paper are NCBI, KEGG, BLAST, MULTALIN, PHYLIP.After tracing phylogeny of enzymes involved in anthracene degradation pathway,both the enzymes showed ancestral relationship with Oriya sativa. Therefore Oryza sativa can be an alternative source to obtain anthraquinone of plant origin. when phylogenetic relationship for octaketide synthase was traced it showed relationship with pentaketide synthase of Aloe arborescens and chalcone synthase of Naringenin, Hypericum hookerianum, Vitis vinifera and Senna alata and also with aromatic polyketide synthase of Solenostemon scutellarioides. Therefore they can be alternate source to obtain anthraquinones. A list of valuable secondary metabolites and their possible alternative sources is also discussed in the paper.

INTRODUCTION

Anthraquinone (9, 10-dioxoanthracene) is an aromatic organic compound (Figure 1). It has the appearance of yellow or light gray to gray-green solid crystalline powder .L. C. Macleod and C. F. H. Allen (1943). It is used for production of various types of dyes like Alizarin, Anthrapurpurin, Carminic acid, Disperse red 11, Disperse red 9, Purpurin, Quinizarine green SS, Solvent Violet 13 etc (all these dyes have same anthraquinone nucleus but different position and substituted groups like hydroxyl, amine, sugars etc). All these dyes are frequently used in the cosmetics like lipsticks, hair colors, decorative eye cosmetic, nail varnish etc. BioNetmat proposal (1997).

Figure 1

Figure 1- Chemical Structure of Anthraquinone



Anthraquinones naturally occur in some plants (eg. Aloe) fungi, lichens and insects where they serve as a basic skeleton for their pigments. Hegnauer (1959); Thomson (1987); Teusher and Lindequist (1994). Large numbers of dyes are obtained from insects like Galerucinin, Sermylini,

Luperinin species. Hilker and schulz (1991). Due to increase in cosmetic demand, these insects are exploited rapidly to economically obtain dyes from them. But due to awareness caused by animal protection groups and allergies caused by the dyes have drawn the interest of researchers toward the use of anthraquinones of plant origin. BioNetmat proposal (2005)

In plants two main biosynthetic pathways leading to anthraquinone production are

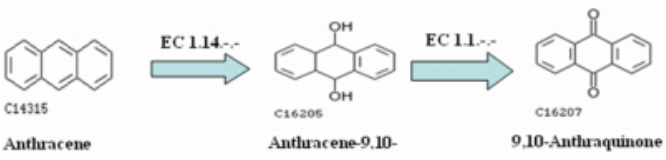
- Shikimate/ Chorismate pathway
- Polyketide pathway.

These pathways are yet not fully understood. The precursors and enzymes involved in these pathways for anthraquinone production are still to be worked out experimentally.

Anthraquinone is a derivative of anthracene, it belongs to the family of polycyclic aromatic hydrocarbons and is not a friendly chemical. It is a severe irritant and sensitiser, both to the skin and eyes, and when taken orally it causes severe damage to the liver, kidneys and mucous membranes. Upon inhalation, severe lung damages occur so anthraquinone production in laboratories is risky. Hans & Elzbieta Brand (2006).Therefore anthracene degradation pathway can be an approach to predict new sources for production of anthraquinone in plants (Figure 2). The anthracene degradation pathway involves two enzymes. Oxidoreductase (EC 1.14.-.-) acting on paired donors with incorporation of molecular oxygen and Oxidoreductase (EC 1.1.-) acting on CH-OH groups of donors.

Figure 2

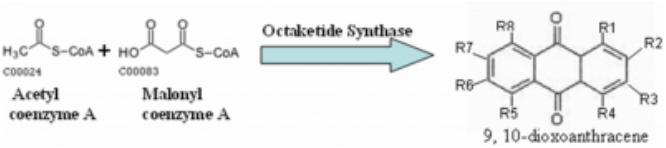
Figure 2- Anthracene Degradation Pathway obtained from KEGG



Recently Scientists have proved that octaketide synthase is responsible for anthraquinone production in plants. Abe et al. (2005), Morita et al. (2007). (Figure 3)

Figure 3

Figure 3- Anthraquinone Production in plants by octaketide Synthase obtained from KEGG

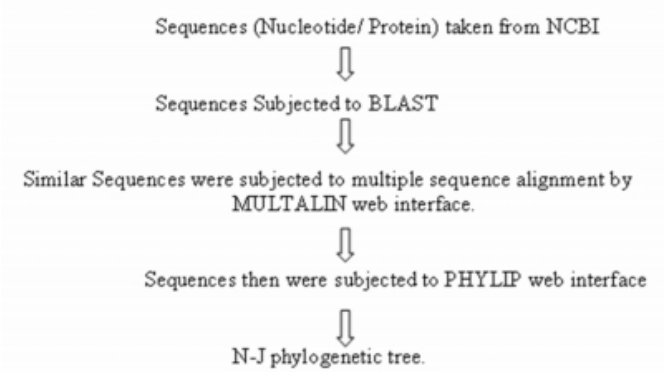


In this paper an attempt has been made to predict alternative source for anthraquinone mainly of plant origin, so as to conserve the insects from exploitation and extinction through Bioprospecting. It is one of the prominent areas of research of commercial important compounds, which is not only providing alternative source for these compounds but also improving the quality of products and cost effective extraction. In the present study enzymes involved in anthracene degrading pathway and octaketide synthase are selected to look for plant based anthraquinones.

MATERIAL AND METHODS

The nucleotide sequences of all enzymes involved in the pathways were taken from NCBI- GenBank and KEGG. The most similar sequences for each enzyme were searched through BLASTn. Now, the most similar sequences for all enzymes were collected and multiple sequence alignment for all of the enzymes were done using MULTALIN web interface. PHYLIP web interface was then used to generate the outtree files in newick format using neighbor joining method through neighbor program.

Figure 4



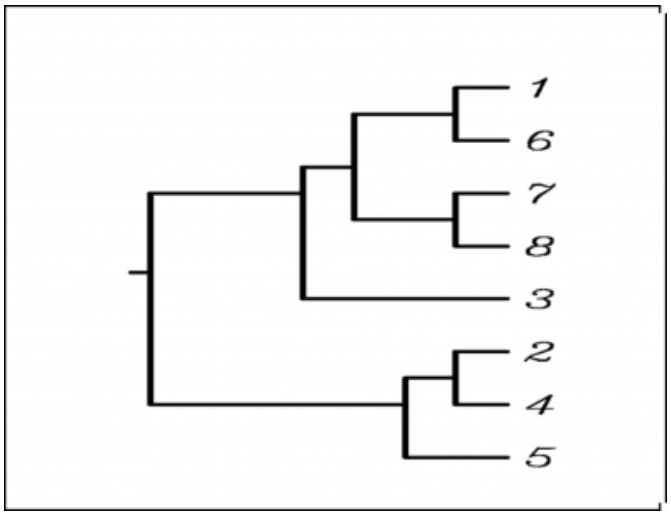
RESULTS AND DISCUSSION

Oxidoreductase; acting on paired donors with incorporation of molecular oxygen (EC 1.14.-.-) was found in Solanum tuberosum, Solanum lycopersicum, Oryza sativa, Ornamental tobacco, Nicotiana benthamiana, Lycopersicon esculentum, Pisum sativum and Citrus sinensis. Among them Oryza sativa, Pisum sativum, Lycopersicon esculentum

and Solanum tuberosum were closely related, whereas Solanum lycopersicum and Nicotiana sp. showed neighbour relationships.(Figure 4)

Figure 5

Figure 4- N J tree for Oxidoreductase (EC 1.14.-.-)



Potato stolon, Cornell University Solanum tuberosum cDNA

Tomato nutrient deficient roots Solanum lycopersicum cDNA clone

Drought Stress Panicle Library Oryza sativa Indica Group cDNA clone

Ornamental tobacco (LxS8) post-fertilization Floral nectary cDNA library Nicotiana langsdorffii x Nicotiana sanderae cDNA clone .

Nicotiana benthamiana cDNA clone

Lycopersicon esculentum clone 133672F, mRNA sequence.

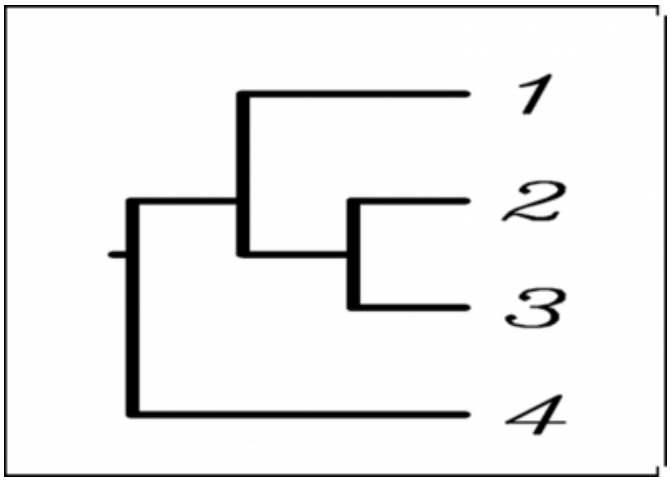
Pisum sativum CYP90A mRNA

Citrus sinensis cytochrome P450 mRNA

Oxidoreductase; Acting on CH-OH groups of donors (EC 1.1.-) was found in Oryza sativa species. (Figure 5). This enzyme was present in different varieties of Oryza Sativa.

Figure 6

Figure 5 N J tree for Oxidoreductase (EC 1.1.-)



Oryza sativa (japonica cultivar-group) genomic DNA, chromosome 4

Oryza sativa genomic DNA, chromosome 4,

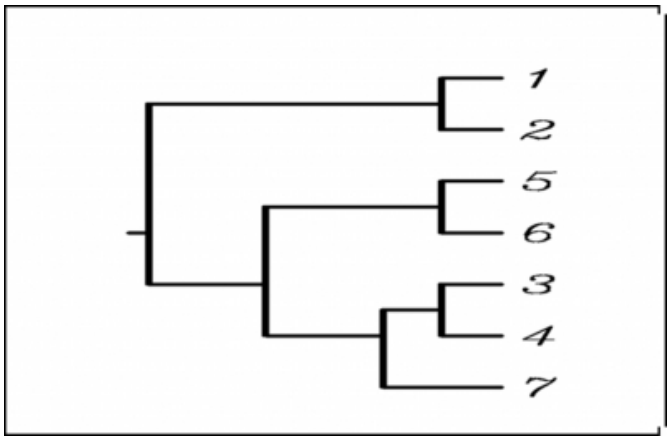
Oryza sativa genomic DNA, chromosome 4, BAC clone

Oryza sativa (japonica cultivar-group) cDNA clone

Octaketide synthase enzyme experimentally obtained only from Aloe arborescens showed anscestral relations with pentaketide synthase of same plant and neighbourhood relationship with Naringenin-chalcone synthase, Hypericum hookerianum-laromatic polyketide synthase, Solenostemon scutellarioides- chalcone synthase, Vitis vinifera- chalcone synthase and Senna alata- chalcone synthase.(Figure 6)

Figure 7

Figure 6- NJ tree for octaketide synthase



Octaketide synthase [Aloe arborescens].

Pentaketide chromone synthase [Aloe arborescens]

Chalcone synthase (Naringenin-chalcone synthase).

Aromatic polyketide synthase [Hypericum hookerianum]

Chalcone synthase [Solenostemon scutellarioides]

Chalcone synthase [Vitis vinifera]

Root-specific chalcone synthase [Senna alata]

CONCLUSION

Since both the enzymes of Anthracene degradation pathway to obtain Anthraquinone, were present in Oryza sativa, therefore Oryza sativa can be an alternative source to obtain anthraquinone of plant origin.

On the other hand the enzyme Octaketide synthase responsible for anthraquinone production in plants present in Aloe arborescens also showed ancestral relationships with the pentaketide synthase of same plant and neighbour relationship with chalcone synthase of Naringenin, Hypericum hookerianum, Vitis vinifera and Senna alata and also with aromatic polyketide synthase of Solenostemon scutellarioides. Therefore Naringenin, Hypericum hookerianum, Vitis vinifera and Senna alata and Solenostemon scutellarioides can be alternate source to obtain anthraquinones.

Applying the same methodology a list of alternative source of various valuable compounds is also given. An attempt has been made to find alternative sources for 14 different valuable compounds from terpenoid (3), diterpenoid (2), indole & ipacac alkaloid (5), phenyl propanoid biosynthesis (5) pathways

Figure 8

Table-1 shows list of secondary metabolites and their possible alternative sources

Pathway for the synthesis of Secondary Metabolites

Alkaloid	Alternative sources
Terpenoid Biosynthesis Pathway	
strictosidine	*Arabidopsis thaliana, Chlamydomonas reinhardtii, Oryza sativa*
cadinene	*Oryza sativa, Arabidopsis thaliana*
vetispiradiene	*Arabidopsis thaliana*
Diterpenoid Biosynthesis Pathway	
Aconitin	*Arabidopsis thaliana, Brassica rapa subsp, Zea mays, Oryza sativa*
Indole & Ipacac Alkaloid Biosynthesis Pathway	
Serpentine	*Oryza sativa,Catharanthus roseus , Rauvolfia serpentina .*
sarpagine	*Nicotiana tabacum ,Catharanthus roseus , Rauvolfia serpentine*
Raucaffricine	*Vitis vinifera, Nicotiana tabacum, Arabidopsis, Rauvolfia serpentine.*
ajmaline	*Vitis vinifera, Nicotiana tabacum, Arabidopsis, Catharanthus roseus , Rauvolfia serpentine.*
vincristine	*Vitis vinifera, Catharanthus roseus Solanum tuberosum., Arabidopsis thaliana.*
phenyl propanoid Biosynthesis Pathway	
Coumarine	*Capsicum chinense, Arabidopsis thaliana*
cinnamaldehyde	*Lithospermum erythrorhizon,Rubus idaeus, Populus balsamifera,*
pinosylvin	*Pinus sp., Abies alba*
ferulic acid	*Pinus taeda,Populus sp., Nicotiana tabacum, Vitis vinifera, Ammi majus*
scopolamine	*Solanum sp., Atropa sp., Brassica juncea,Cicer arietinum, Pisum sativum*

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