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Dr. Gorakh Nath Tiwari
Secretary & Editor

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Certificate of Publication

This is to certify that the Research Article named **Hindi Patrakarita Kaa Badalta swaroop** is published in our Quarterly magazine on April.-Sept., 2018 (Year 46, Joint Edition-2&3) of Dr. shashikant Mishra.

We seek your kind co-operation in future.

(Dr. Gorakhnath Tiwari) 12.10.2018

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This is to certify that the A Interview Of Prof. Ramkumar Mishra (International Economist & Director IPE, Hyderabad) is taken by Dr. Shashikant Mishra for our Quarterly Magazine. This Interview Named **"Prof. Ramkumar Mishra se Dr. Shashikant Mishra ki Khas Batchit"** is Published in Oct.-Dec., 2018, Year-46, Edition-4.

We seek your kind co-operation in future.

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FLIPPED CLASSROOMS: ADVANTAGES AND DISADVANTAGES

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Abstract:

Flipped learning is a pedagogical approach in which the conventional notion of classroom-based learning is inverted, so that students are introduced to the learning material before class, with classroom time then being used to deepen understanding through discussion with peers and problem-solving activities facilitated by teachers. In traditional style teacher focuses on explaining the content using a lecture method. Student engagement in the traditional model may be limited to activities in which students work independently or in small groups on an application task designed by the teacher. Class discussions are typically centered on the teacher, who controls the flow of the conversation. In a Flipped classroom students are actively involved in knowledge acquisition and construction as they participate in and evaluate their learning. Efficient use of flipped classroom allows most students to do a year's work in much less time. Advanced students work on independent projects while slower learners get more personalized instruction. Some students might not get through the year's material, but demonstrated competence on the parts they did complete. My paper discusses merits and limitations in using flipped class technologies; and would the share the experience of the flipped class techniques followed in our class.

Key Words: Flipped Classrooms, Student Centered Learning, Knowledge Acquisition, Deep Understanding & Project Based Learnings.

Introduction:

In the present world of globalisation and in the 21st century senario technology has opened the doors of innovation in various fields and mainly in education. In recent times Flipped classrooms are playing vital role in teaching learning process. These classrooms throw a challenge to traditional classroom procedure. Flipped classrooms provide great scope for learners to enrich themselves with many skills which at large would help them be ready for the industry. The revolution of flipped classrooms help teachers to use their time in being more creative and proactive. They become more accessible to the slow learners and can motivate them in activities and tasks. The flipped classrooms assist in promoting a teacher's role from instructor to a guide, coach and a fecilitator. Teacher can motivate students to have deep knowledge on concepts and further help them to cultivate skills which would eventually lead to their empowerment.

The traditional methods of teaching and learning would encourage students to always depend on teacher and knowledge of concepts and theories would be limited. Students would find it difficult to complete the homework as they had to depend on teacher's lecture; which hardly allowed some students to grasp the lesson for the first time. In traditional classroom atmosphere students face problems of doing many things at a time like: listening to lecture, taking down notes and completing the worksheet. These classes gave less importance to creativity of students. But, in flipped classroom students learn the concepts, ideas before coming to class, depending on the suggestions given by teacher. It was teacher's responsibility to ask them to watch few videos, online ppts, podcasts, blogs and other web tools. At the same it was inevitable for teacher to do some research on all possible web tools; in order to be proactive.

In the present paper I would like to share some experiences of experimenting a flipped classroom technique in a English language class in our college. The first year undergraduate students were given 10 topics from Adous Huxley's prose "Benaras." Each topic was divided into 3 sub topics. Every student was given a topic, students were asked to collect information about the topic and each team had 3 members. They were suggested to use online sites, google down information or watch videos on you tube or take help from blogs. They had to write down few sentences and collect pictures about the topic and share the information with team mates. Later they took turns and explained about their research to the whole class. Finally they read the prose text and completed the task on reading comprehension. Whenever they found it difficult to comprehend I assisted them with hints and clues. I could interact and closely observe students working in teams. To my surprise each one was interested in completing all stages of work and was excited to be a part of whole process. They got a chance to learn deeply about each topic which made their interaction more interesting.

There are Many Advantages of Flipped Classrooms:

- ✓ Encourages Spirit of Research in Students: In flipped classroom students get to see what everybody else has seen and think what nobody else has thought. Teacher allots some concepts to students in class which they go home and find about those concepts by themselves .They make notes in their own style which paves way to original and unique understanding.

- ✓ Liberation in Homework: The flipped classroom technique gives ample scope for students to make their own choice of expressing views on the given concept. They get to watch, read and observe videos, information which gives them freedom to make notes. Previously students who took running notes which would always have a risk of missing points. But now students can pause, rewind and save the information to carry to class or for further use.
- ✓ Develops Collaborative Work Culture: Unlike traditional learning, in a flipped classroom students share the information they collect with their class mates. Eventually this technique encourages peer learning, project based learning etc. which encourages slow learners to learn and participate in sharing their views by putting aside their inhibitions. They are kept busy with the activities and tasks; moreover they get to seek help and personal attention from the teacher who was not approachable otherwise. The flipped classroom gives more freedom to teachers to zero on how much time to spend with each student. Struggling students, great performers, introverted kids, etc; can get the attention each of them need. In this case, a teacher gets chance to observe the students pace of learning and frames the instructions accordingly. The flipped class caters to the needs of irregular students who can catch up with the peer group faster and learn easily.
- ✓ Student Centered Classroom: The classrooms shifts focus from teacher needs to student needs as it stresses on student centred teaching approach. Teacher makes use of time in classroom by supporting students in grasping the concepts through practical application and giving hands on experience as they already have an idea of the concept.

The flipped classroom inspires teachers to offer a versatile and engaging way to share learning content, while shouldering more responsibility on students regarding their own career. At work place like-minded teachers can share resources, tips, to make successful flipped classrooms. While this model of education has not spread in each and every classroom yet, it seems like it's going there.

Limitations in Using Flipped Classrooms:

Flipping classrooms is inspiring teachers to change the way they've always done things, and it is motivating them to bring technology into their classrooms through the use of video and virtual classrooms.

- ✓ More Workload on Teachers: Teacher needs to spend more time in planning her lessons as each individual student has viability to watch various videos and tools. She must put in extra effort to make activities and tasks which would test the potential of all kinds of learners. Students show their mastery of content the way they like. "Are we doing things differently or doing different things?" As educators around the globe try to flip their class, it's an important thing to reflect on.
- ✓ Technical Issues: Access to internet is a must if students want do their projects and homework. Lack of technical knowledge or technology means no work or progress. There is another threat that students may spend more time in front of the screens and there is possibility of getting distracted.
- ✓ Initial Set Up Needs More Time: The teacher need to plan, organise and implement their lessons, task and activities in such a way that students find it interesting .In case of lack of technical knowledge or if students are unable to catch up with teacher's guidelines the whole purpose of it would be lost. The students need to have zeal to do new things. Only in few urban areas it would be possible to experiment. The standard and socio economic background of the student and teacher plays a vital role. Thus teacher needs to be more patient in working out things.
- ✓ Interest of Students: If students drop the idea of doing homework there is no room for flipped class. Teachers creativity primarily needs to focus on motivating students to do their homework.
- ✓ Not Every Ones Cup of Tea: The flipped classroom method would be more apt for self disciplined and self motivated students. Students should have good knowledge in coping with technical problems too, on the other hand in case of failure to complete the homework; it would demotivate the students further. It consumes more time for students to realise as to how they accustom with the new approach.
- ✓ Highly Expensive and Risky: In case of implementing flipped classrooms one needs to be financially ready to bear the cost of installing devices, projects, new curriculum and training the teachers in skills needed. The managements need to plan and decide on issues like at what level of teaching and which subjects and curriculum can be suitable for flipped class.
- ✓ Change May be a Bitter Pill: Teachers who though are aware of the drawbacks of traditional methods still don't mind carrying it but this change requires lot of efficiency, patience, willings to accept the change and self motivation. The teachers themselves need a lot of training in order to equip themselves with new trends in teaching and embrace innovative techniques. The more challenging role a teacher needs to play is with same amount of exuberance teacher requires to motivate students. Further there is still a doubt if one would be sure of accomplishing the targeted goals.

Conclusions:

The combination of flipped classroom with the just in time teaching approach may be a useful union to assist students to clear confusing material and develop deep learning strategies. It also helps in independent learning. There is no doubt that in present generation students are learning to work on projects, experiments,

activities to understand the concepts in various fields. The new approach may have some limitations but one must try to gain from the benefits of flipped classroom method in one way or the other. Whenever the teacher can implement this new approach it must be followed as this method needs more time to become user friendly. The other traits a student enriches shouldn't be left unseen; it promotes multi tasking, interpersonal skills, decision making skills and problem solving skills, on whole these skills would make the students equip for empowerment.

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ARTICLE

WILEY

Synthesis, kinetics, and mechanism of bromophenols by *N*-bromophthalimide in aqueous acetic acid

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Abstract

The kinetics and mechanism of bromination of phenol and its substituents, viz. 4-chlorophenol, 4-bromophenol, 4-methylphenol, and 4-methoxyphenol by *N*-bromophthalimide (NBP) in the presence of mercuric acetate in the temperature range of 303–318 K in aqueous acetic acid medium have been investigated. The reaction follows first-order dependence on [NBP] and fractional order dependence of rate on [Phenol]. The activation parameters have been evaluated, and based on the observed kinetic results the probable mechanism has been proposed. Observed kinetic features and Hammett's reaction constant (ρ) suggests that bromination occurs through electrophilic substitution of bromonium ion (Br^+) into the aromatic ring in the transition state. Large negative entropy of activation values probably suggests the rigid nature of transition state.

KEYWORDS

bromination, kinetics, *N*-bromophthalimide, phenols

1 | INTRODUCTION

Bromination of aromatic compounds received evergreen interest for the past several decades, because a large numbers of brominated aromatics are used as key intermediates or precursors during the synthesis of agrochemicals, pharmaceuticals, and organometallic compounds.[1–5] In the earlier years, molecular bromine was the most commonly used reagent to achieve bromination. But this reagent is not only toxic but also hazardous and releases corrosive HBr as the side product. If due care is not taken during its use, skin burns may occur. To overcome these issues, a "brominating mixture (bromate–bromide reagent)" is being used along with mineral acid for the in situ generation of either molecular bromine or tribromide ion (Br_3^-) to afford bromination. However, these methods are also associated with the excess of unused acid and HBr which will be sent into the laboratory/industrial wastes.[6] With a view to overcome toxicity issues ,considerable attention has been focused on N-halo compounds (>N–X)[7–12] for halogenation and oxidation due to their ability to act as a source of halonium cations (X^+), and hypohalite (OX^-) species. During the past several decades, *N*-bromocompounds, such as *N*-bromosuccinimide (NBS), *N*-bromoacetamide, and *N*-bromophthalimide (NBP) are most commonly used in bromination reactions, which could prevent the toxicity and acid waste.[7–12] However, in recent past, NBP is preferred over NBS owing to its high stability. A perusal of literature shows few interesting reports on oxidation kinetics,[13] but not many reports are available on the potential application of NBP as a brominating agent. Nevertheless, in a recent publication we have studied NBP triggered bromination of aromatic compounds in the presence of aqueous acetic acid. Reaction kinetics indicated first order in [NBP] and zero order in [Anisole]. The reactions afforded very good yields of corresponding bromo derivatives under kinetic conditions. The mechanism of the reaction is explained through the formation of acetyl hypobromite due to the interaction of NBP and acetic acid, which in turn reacts with anisole to afford bromo derivative of anisole.[14] Encouraged by these results, we have taken up the synthesis of bromophenols by NBP. To gain an insight into the mechanistic aspects, we have studied the kinetics of bromination of phenols using NBP in aqueous acetic acid (Scheme 1).

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Microwave Assisted Synthesis of 1-(Arylthio)naphthalen-2-ols and Their Antimicrobial Activity[1]

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Abstract—A series of 1-(arylthio)naphthalen-2-ols have been synthesized by condensation of naphthalen-2-ol with 1,2-diaryldisulfanes in the presence of iodine under microwave irradiation and conventional heating methods. Structures of the products were elucidated from the spectral data (IR, ^{1}H, and ^{13}C NMR, mass spectra) and elemental analysis. All products were tested for *in vitro* antibacterial and antifungal activities.

Keywords: thionaphthalenes, microwave irradiation, antibacterial and antifungal activity

DOI: 10.1134/S1070363217120337

INTRODUCTION

Naphthalene derivatives play an important role in pharmaceutical industry due to their biological activities, such as antibacterial [1], antifungal [2] and some others. Introduction of sulfur atom(s) in biologically active naphthalene derivatives could enhance their valuable properties. In view of producing potentially biologically active compounds, we have synthesized a number of naphthyl sulfides.

Synthesis of aryl sulfides usually involves such synthetic procedures as dehydrogenative coupling of thiophenols with aromatic compounds and a variety of conventional heating methods. Most of such processes suffer from certain limitations including tough reaction conditions, low yields, tedious work-up procedures, relatively long reaction time, and side reactions. Microwave assisted synthesis could be an alternative green approach to the target compounds [3].

RESULTS AND DISCUSSION

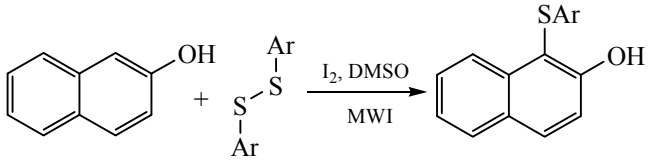
As a part of our ongoing research in eco-sustainable synthesis of organic compounds [4,5], herein we present the synthesis of 1-(arylthio)naphthalen-2-ols induced by microwave irradiation (Scheme 1 and table).

According to the data presented in the table, the microwave irradiation approach to the synthesis of 1-(arylthio)-naphthalen-2-ols was much more efficient than the one carried out upon conventional heating. It proceeded much faster giving somewhat higher yields of the products, presumably without side reactions.

Antibacterial activity. All products were screened for their *in vitro* antibacterial activity against *Escherichia coli* and *Staphylococcus aureus* using ampicillin as the standard drug. Activity was determined using the cup plate agar diffusion method by measuring the zones of inhibition in mm. The compounds were screened at concentrations of 25, 50 and 100 μg/mL in DMSO. According to the screening data it was evident that the synthesized compounds **3d**, **3e,** and **3g** demonstrated high antibacterial activity against all tested organisms.

Antifungal activity. All products were screened for their antifungal activity *in vitro* against *Aspergillus niger* and *Candida metapsilosis* using grieseofulvin as the standard drug. Activity was determined using the cup plate agar diffusion method by measuring the zones of inhibition in mm. The compounds were screened at concentrations of 25, 50 and 100 μg/mL in DMSO. According to the screening data it was evident that the synthesized compounds **3d** and **3e** demon-

Scheme 1. Synthesis of 1-(arylthio)naphthalen-2-ols (**3a–3g**).



1 **2a–2g** **3a–3g**

[1] The text was submitted by the authors in English.

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SECTORAL ALLOCATION OF MF SCHEMES – A STUDY

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ABSTRACT

Mutual Fund Investment is one of the most recommended tool for wealth creation, especially for the salaried middle class. The number of options available too, are mind boggling from an average investors perspective. More often than not, if the scheme belongs to a reputed AMC, the investor rarely looks beyond the returns generated. Historical performance is no doubt important, but there are other aspects too, that can be used to predict returns, one such is the 'sectoral allocation'. In this study an attempt has been made to study the sectoral and stock allocation of select equity growth schemes to study how different these offerings are. Can an investor really look beyond returns, brand names and fund manager? A strong core similarity was found among the schemes in terms of both sector and stock selection. The study also reveals that differences in sector allocations had impacted returns, but this study is only a cross-sectional study, a longitudinal study would be needed to make more meaningful conclusions.

Keywords : Mutual Funds, sectoral allocation, equity growth scheme, historical returns, stock selection, variability.

భాషా పునశ్చరణం... సాహితీ సింహావలోకనం

తెలుగు అధ్యాపకులు భాషా సాహిత్యాలను ఓసారి సింహావలోకనం చేసుకోవడానికి ఉస్మానియా విశ్వవిద్యాలయంలోని యూజీసీ - హెచ్ఆర్డీసీ (అకడమిక్ స్టాఫ్ కళాశాల) పునశ్చరణ తరగతులు నిర్వహించింది. జూన్ 22 నుంచి జులై 12 వరకు జరిగిన వీటిలో తెలంగాణ, ఆంధ్రప్రదేశ్‌లోని యూనివర్సిటీ డిగ్రీ కళాశాలల అధ్యాపకులు పాల్గొన్నారు. బోధనలో స్పృశించాల్సిన అంశాలను వీళ్లకు సూచిస్తూ, భాషాసాహిత్యాల స్థితిగతులను విశ్లేషించిన ప్రసిద్ధ సాహితీవేత్తలు, విషయనిపుణుల ప్రసంగాలు ఆలోచింపజేశాయి.

ఏ రంగంలోని వారైనా అప్పుడప్పుడూ దానికి సంబంధించిన సమస్త విషయాలను సింహావలోకనం చేసుకోవడం తప్పనిసరి. దీనివల్ల ఆ రంగంలో జరుగుతున్న అభివృద్ధి, మార్పుకోసం జరుగుతున్న ప్రయత్నాలు, ఇంకా ఎన్నో ఇతర విషయాల గురించి అవగాహన వస్తుంది. ముఖ్యంగా భావి భారత పౌరులను తీర్చిదిద్దే బోధన రంగంలో ఇది అత్యవసరం. ఈ నేపథ్యంలోనే మూడు వారాల పాటు అకడమిక్ స్టాఫ్ కళాశాల పునశ్చరణ తరగతులు నిర్వహించింది. వీటికి ఉస్మానియా విశ్వవిద్యాలయం తెలుగు శాఖాధిపతి ఆచార్య సూర్యా ధనంజయ్ సమన్వయకర్తగా వ్యవహరించారు.

"అధ్యాపకులకు వినియోగ పాండిత్యం కావాలి. అధ్యాపక వృత్తి నదిలా ఉండాలి. పాఠ్యాంశానికి సంబంధించి ముందే సిద్ధమై వెళ్లిన తరగతి ఎక్కుపెట్టిన బాణం లాంటిది" అన్నారు కేంద్ర సాహిత్య అకాడమీ పురస్కార గ్రహీత, ప్రముఖ కవి డా॥ ఎన్.గోపి. జూన్ 22న తరగతుల ప్రారంభం సందర్భంగా ఏర్పాటు చేసిన సభలో ఆయన కీలకోపన్యాసం చేశారు. దీనికి అకడమిక్ స్టాఫ్ కళాశాల సంచాలకులు ఆచార్య ఎ.బాలకిషన్ అధ్యక్షత వహించారు. ముఖ్య అతిథి, ఉస్మానియా విశ్వవిద్యాలయం ఉపకులపతి ఆచార్య రామచంద్రం పునశ్చరణ తరగతుల ప్రాముఖ్యాన్ని, అకడమిక్ స్టాఫ్ కళాశాల ప్రత్యేకతను వివరించారు. ఆ తర్వాతి రోజు నుంచి విషయ నిపుణుల ప్రసంగ పాఠాలు ప్రారంభమయ్యాయి.

సంస్కృతికి శ్వాసనాళాలు శాసనాలు

వేమన, వీరబ్రహ్మంలతో సామాజిక ఉద్యమాలు ప్రారంభమయ్యాయని, కులం లేని సమాజాన్ని నిర్మించడమే వీటి లక్ష్యమని చెప్పారు పాత్రికేయులు జూలూరి గౌరీశంకర్. 'సామాజిక ఉద్యమాలు-కవిత్వం' అంశం మీద ఆయన మాట్లాడారు. 'లము కవితా రూపాలు - అభివ్యక్తి వైవిధ్యం' అంశం మీద కవి, విమర్శకులు డా॥ అమ్మంగి వేణుగోపాల్ ప్రసంగించారు. హైకూ, నానీ, మినీ కవిత, రెక్కలు కవితా ప్రక్రియల్లోని అభివ్యక్తి వైవిధ్యాన్ని వివరించారు. తెలంగాణ బీసీ కమిషన్ అధ్యక్షులు బి.ఎస్.రాములు 'నా కథ- నేపథ్యం' మీద మాట్లాడుతూ.. కథలో హృదయావిష్కరణ జరగాలన్నారు. విమర్శకులు ఆచార్య రాచపాళెం చంద్రశేఖరరెడ్డి 'తెలుగు కథ- సామాజిక పరిణామాలు', 'విమర్శ పద్ధతుల' మీద ప్రసంగించారు. తెలుగులో ఇప్పటివరకూ రెండు లక్షల కథలు వచ్చాయని, 90 శాతం కాలక్షేపం కథలు పోగా, మిగిలినవే జీవితాన్ని చిత్రించాయన్నారు. దశలవారీగా తెలుగు కథానిక పరిణామాన్ని వివరించారు. పాఠకునికి, రచయితకు మధ్య వారధి విమర్శకుడని చెప్పారు. సాహిత్యకారుడి కంటే విమర్శకుడు ఎక్కువగా చదవాలని పేర్కొన్నారు. కథకులు పెద్దింటి అశోక్‌కుమార్ 'ఆధునిక తెలంగాణ కథ', 'కథన పద్ధతులు' అంశాల మీద మాట్లాడారు. 1970 నుంచి 2000 వరకు వచ్చిన తెలంగాణ కథ వైవిధ్యాన్ని,

వ్యాస రచనలో భాషా వినియోగం

డా॥ చంద్రయ్య .ఎస్

ఉపోద్ఘాతం:

ఆధునిక కాలంలో వ్యాసం అందరికీ అందుబాటులో ఉన్న సాహిత్య ప్రక్రియ. ఇది సృజనాత్మకమైందీ; బౌద్ధికమైంది. తెలుగునాట వివిధ పత్రికల్లో ప్రతిరోజు కనీసం మూడు వందలకుపైగా వ్యాసాలు వస్తున్నాయని ఒక అంచనా. వ్యాస రచనకు మాత్రమే కాదు-ప్రతి రచనకూ నిర్దిష్ట పాఠకులు ఉంటారు. రచయిత ఎంచుకున్న అంశం, లక్షిత పాఠకులు, రచయితకున్న భాషా సంపద, రచయిత సామాజిక నేపథ్యం మొదలైన కారణాలు ఒక రచనలో ఉపయోగించాల్సిన భాషను నిర్దేశిస్తుంటాయి. అయితే, మిగతా ప్రక్రియల రచయితలకంటే, వ్యాస రచయితలపై ఎక్కువ సామాజిక బాధ్యత ఉందనేది వివిధ పత్రికల్లో వెలువడుతున్న వందలాది వ్యాసాలు గుర్తుచేస్తున్నాయి. ఇంత విస్తృతంగా ఉపయోగంలో ఉన్న వ్యాస ప్రక్రియలో ఉపయోగించవలసిన భాష విషయంలో కొన్ని ఆలోచనలను మీతో పంచుకోవాలని ఈ వ్యాసం రాశాను. తెలుగునాట ప్రత్యామ్నాయ భావజాలాన్ని వ్యాప్తిచేస్తున్న కొన్ని పత్రికల్లో ఉపయోగించిన భాష ఆధారంగా ఈ వ్యాసం రూపొందించాను.

'నాకు, మీలాగా పదాలపై పట్టులేదు. కవిత్వ భాష తెలియదు.' అనే మాటలను మనం తరచూ వింటూ ఉంటాం. ఇదే అభిప్రాయం వ్యాస రచన విషయంలోనూ, భాషావ్యవహర్తల్లో ఇటువంటి అభిప్రాయాలు ఏర్పడటానికి 'నాన్యషి కురుతే కావ్యం', 'కవిరేవ ప్రజాపతిః' వంటి మాటలు మన అధ్యయన, అధ్యాపనలను ప్రభావితం చేయడం కారణం. ఈ వాఖ్యలను మరింత వివరంగా అర్థం చేసుకోవాల్సి ఉంది. కవి/రచయిత సాధారణ ప్రజలతో, వారి భాషతో సంబంధాన్ని తెంచుకుంటేనే గొప్పవ్యక్తిగా కీర్తించబడుతాడేమోననే ఒక దురభిప్రాయం చారిత్రకంగా బలపడుతూ వచ్చింది. కనుక, ప్రజలకు అర్థమయ్యే భాషను వాడితే తనకు ప్రత్యేకత ఏముంటుంది అనే మానసిక స్థితికి ప్రాధాన్యత పెరుగుతూ వచ్చింది. ఈ రకమైన దురభిప్రాయం జన సామాన్యమైన వ్యాసరచనలోనూ ప్రవేశించింది. కనుక, రచయితల్లో కొందరు 'ప్రజలకు అర్థంకాని భాష వాడుతున్నారు' అని అనలేం. కానీ, కష్టపడితే కానీ అర్థంకాని పదజాలం వాడటాన్ని మాత్రం గమనిస్తూనే ఉన్నాం. గ్రాంథిక భాష వాసనలను ప్రయత్నపూర్వకంగానైన వదిలించుకోలేనితనాన్ని గుర్తించవచ్చు. ప్రత్యేకత కోసం పాకులాటలో ఇంతకాలం ప్రజలకు అర్థంకాకుండా ఉండటానికి రచయిత ఎంత కష్టపడుతూ వచ్చాడో, ఇప్పుడు ప్రజల భాషకు కట్టుబడి, కష్టపడి రాయాల్సిన అనివార్యత ప్రజా రచయితల ముందుంది. "వ్యాసకర్త కష్టపడితే పాఠకులు సుఖపడతారు, వ్యాసకర్త శ్రమ పడకపోతే ఆ మేరకు పాఠకులు శ్రమ పడాల్సి వస్తుంది."(చెంచయ్య, వి. 2009:16) అనే పరిశీలన యథార్థం.

"వ్యాసానికి సంబంధించిన భాష సరళంగా ఉండాలి. శైలి చదివించేదిగా ఉండాలి. భాష ఇలా ఉండాలనీ, ఇలా ఉంటుందనీ చెప్పొచ్చుగాని, శైలి ఇలా ఉంటుందని చెప్పలేం. ఎవరి శైలి వారిదే. భాష ద్వారా రచయిత భావాలు మాత్రమే వ్యక్తం అవుతాయి. శైలి ద్వారా రచయిత వ్యక్తిత్వం కూడా వ్యక్తం అవుతుంది. భాష మేఘం అయితే, శైలి మెరుపు. భాష శరీరం అయితే శైలి ప్రాణం. వ్యాసానికి భాష, శైలి రెండు కళ్లు. వాటి ద్వారానే వ్యాసంలోని విషయాన్ని సరిగ్గా చూడగలం. భాష దెబ్బతిన్నా, శైలి బలహీనంగా ఉన్నా చూపు దెబ్బతిని పాఠకుల మనసుకు విషయం ఎక్కదు." (చెంచయ్య, వి. 2009:20).

రచయితలు వ్యాస రచనలో ఉపయోగించే భాషలో సాధారణంగా చేస్తున్న పొరపాట్లు ఈ కింది విధంగా ఉంటున్నాయి. వీటిని పొరపాట్లు అనికూడా అనలేం. రచయిత రాసేటప్పుడు కొంత శ్రద్ధపెట్టి ఉపయోగించిన భాషను భాషా విషయక దృష్టితో సరిచూసుకొంటే సరిపోతుంది.

1. క్రియా విశేషణాల వాడకంలో పొరపాట్లు
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5. లిఖిత భాషకు, మౌఖిక భాషకు మధ్యగల భేదాలను గుర్తించకపోవడం
6. కర్త, క్రియల మధ్య సమన్వయ లోపం
7. సుదీర్ఘ వాక్యాల రచన

అంతర్జాతీయ తెలుగు భాషాశాస్త్ర పత్రిక

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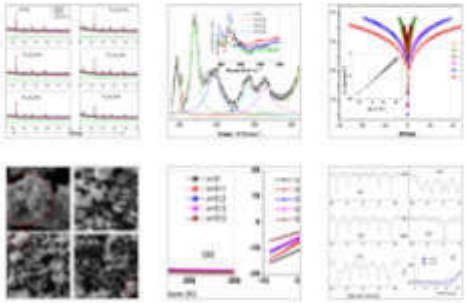
విషయసూచిక పుట

Figures (6)



Tables (2)

Table 1
Table 2

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The electrical, magnetic and ^{57}Fe Mössbauer studies of Al doped $PrFeO_3$ polycrystalline materials

J. Ramesh [a], S.S.K. Reddy [d], N. Raju [a], M. Sreenath Reddy [b], Ch. Gopal Reddy [a], P. Yadagiri Reddy [a] ✉, K. Rama Reddy [a], V. Raghavendra Reddy [c]

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https://doi.org/10.1016/j.ceramint.2018.07.159

Abstract

The structural, electrical, magnetic and ^{57}Fe Mössbauer studies of sol-gel synthesized polycrystalline $Pr_{1-x}Al_xFeO_3$ (x=0, 0.1, 0.2, 0.3, 0.4 and 0.5) samples are reported in this paper and the phase purity of the materials was confirmed from Rietveld refinement of XRD pattern. From the magnetization studies it is observed that the Al doping at Pr site changed the magnetic ordering of the system at both room and low temperatures. The observed isomer-shift values from room temperature Mössbauer spectroscopy confirmed the charge state

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"Designing of Potent Drug to Target Alpha Synuclein in Parkinson's Disease"

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Corresponding Author: E-mail ID: jaganannareddy@gmail.com; +919440350514.
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***Abstract**: Parkinson disease is a chronic and progressive neurodegenerative disorder characterized by muscle rigidity, tremor and bradykinesia. The central aspect of Parkinson disease involves dysmetabolism of specific proteins resulting in aggregation, aborted protein degradation and/or formation of Lewy bodies. Parkinson disease involves the progressive loss of dopamine-containing neurons from the substantia nigra. The study of involvement of a protein named alpha synuclein in disease and the ligands targeting it, to possibly find a drug to cure the disease. Mutation in α-synuclein can lead to misfolding, aggregation and resistance to protein degradation. In silico approach to design a drug for Parkinson's disease is employed to obtain the outcome. Alpha synuclein (PDB id :1XQ8) ,the receptor molecule, is docked with the ligands that sustained the screening procedure exerted by the software suite. Ligands are screened on the basis of numerous criteria such as hepatotoxicity, absorption level, carcinogeniticity and so on. The drug with the lowest docking energy is considered ideal. It may be chosen for further clinical trials and can finally go for FDA approval.*

***Keywords:** Parkinson disease , Alpha synuclein, Docking, ADME/Tox,*

Date of Submission: 02-11-2017 Date of acceptance: 16-11-2017

I. Introduction

Parkinson's disease is a degenerative disorder of the central nervous system. It results from the death of dopamine-containing cells in the substantia nigra, a region of the midbrain; the cause of cell-death is unknown. Early in the course of the disease, the most obvious symptoms are movement-related, including shaking, rigidity, slowness of movement and difficulty with walking and gait. Later, cognitive and behavioural problems may arise, with dementia commonly occurring in the advanced stages of the disease. Other symptoms include sensory, sleep and emotional problems.

PD is more common in the elderly with most cases occurring after the age of 50. Parkinson's disease is often defined as a parkinsonian syndrome that is idiopathic (having no known cause), although some atypical cases have a genetic origin. Many risk and protective factors have been investigated: the clearest evidence is for an increased risk of PD in people exposed to certain pesticides and a reduced risk in tobacco smokers. The pathology of the disease is characterized by the accumulation of a protein called alpha-synuclein into inclusions called Lewy bodies in neurons, and from insufficient formation and activity of dopamine produced in certain neurons of parts of the midbrain. Diagnosis of typical cases is mainly based on symptoms, with tests such as neuroimaging being used for confirmation. Estimates suggest that approximately 750,000 Americans have PD.

Signs and symptoms

Numerous symptoms are witnessed in Parkinson's disease. The various signs and symptoms are Motor Symptoms-Cardinal,Non motor symptoms- Neuropsychiatric ,Sleep,Autonomic, Gastro intestinal , Neuro- opthalmological

Diagnosis

Parkinson's disease is diagnosed by a careful neurological examination, testing movements, coordination, reflexes, and other aspects of function. Several specialized tests may be used, including imaging of the brain with magnetic resonance imaging (MRI) or positron emission tomography (PET). These are not essential to diagnosis in most cases, but may help to confirm the diagnosis in difficult cases and to distinguish PD from similar diseases such as progressive supranuclear palsy.

In-silico approach opens up the perspective to target the particular protein that plays a crucial role in the causation of PD. The major protein involved in the disease is **alpha-synuclein.** Alpha-Synuclein is a 140 amino acid protein abundantly expressed in presynaptic terminals of vertebrates. One of its normal functions is

to regulate dopamine transporter activities as shown in **Fig 1** .This protein contains an NAC region that is prone to aggregate, especially under oxidative stress. The aggregated a-synuclein can inhibit the function of 26S proteasome which is important for the clearance of misfolded proteins and other target molecules. The dysfunction of proteasome will contribute to cell death. Two mutations, A53T and A30P, in a-synuclein have been identified in families with early-onset familial Parkinson's disease. These mutations may accelerate the aggregation of a-synuclein.

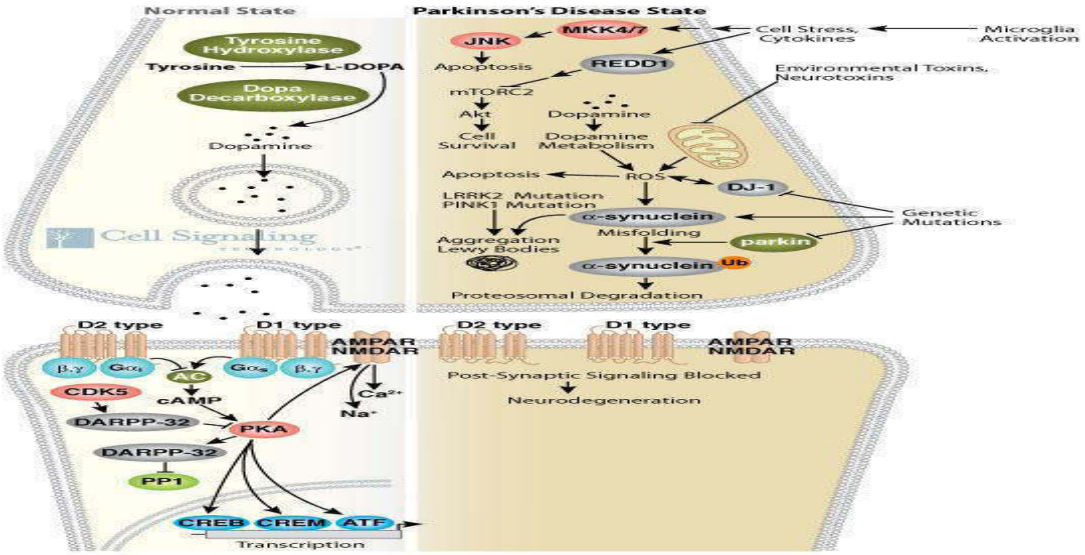

Fig 1

II. Experimental

Protein analysis

Proteins involved in disease are explored through **GeneCards**(provided gene-centric information, automatically mined and integrated from a myriad of data sources) and the most commonly diagnosed protein (alpha synuclein) is selected .The sequence, function and structure of alpha-synuclein is extracted from **NCBI**. **BLAST** is performed employing numerous model organisms. BLOSUM matrix used in BLAST is in accordance with the hierarchy of organisms i.e. BLOSUM 80 with higher vertebrates, BLOSUM 62 with invertebrates and lower vertebrates and BLOSUM 45 in case of microbes. Evolutionary relatedness of model organisms to the query protein is estimated with the help of **SDSC Biology Workbench (**The SDSC Workbench is a web-based tool for biologists that allows to search many popular protein and nucleic acid sequence databases) .Color coded representation of the phylogenetic tree can also be obtained in the form of texshade and boxshade. Conformatory tools like SOPMA, PROTPARAM, PHYRE, JPred, CPH Model were used to derive the structurally based information of the query protein. PDB ids are validated through different tools and the pdb id 1XQ8 is confirmed. So **1XQ8** is found to be the receptor protein.

Simulation of Receptor

Energy minimization of receptor takes place in **Accelrys Discovery Studio** is a software suite of life science molecular design solutions for computational chemists and computational biologists that makes it easier to examine the properties of large and small molecules, study systems, identify leads and optimize candidates). Binding site of the receptor (1XQ8) is edited and charmM and forcefield is applied. Algorithm used in minimization process is Conjugate Gradient. Steps are increased with an increment of 200 until the energy stabilizes. The final value of energy of receptor after minimization is: -6886.47162 kcal/mol.

Creation of library of compounds and Virtual Screening

Myriad of compounds are selected from natural sources and GeneCards. Reviewing the literature and related articles about the disease and treatment assists in selecting the compound from natural sources. The chosen compounds are enlisted and then screened on the basis of Lipnk. 5 Rule.(Bioassay Activity).

ADME Test/TOPKAT on screened compounds

Compounds are screened on the basis of the values of hepatotoxicity and absorption level in ADME in **Accelrys Discovery Studio**. ADME is the test for Absorption Distribution Metabolism Excretion capacities of drugs. If the values of ADMET Hepatotoxicity and ADMET Absorption level are equal to zero, then the compound is selected further for TOPCAT .Non carcinogenicity is the foremost criteria of this screening test. Other parameters are that are considered for testing are**:** Rat Oral LD50, Developmental Toxicity Potential (DTP),

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Medicinal Importance of Plants in the Religious Festivals of Telangana (India)

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Abstract:

Biodiversity an important gift of nature is now under great threat owing to anthropogenic activities. Indians have been worshipping trees since time immemorial and this is done as a matter of gratitude as we know that life cannot exists without trees, hence trees and their products are part of our rituals and ceremonies. A study was carried out to find the importance of plants in religious festivals and in traditional healing system of the people of Telangana region. People of Telangana have a unique culture of worshipping plants in their regional festivals like Bathukamma, Bonalu, Ugadi, Vinayakachavithi etc. It was observed that sacred plants have significant role in rituals as well as in alternative health care system. Ethanobotanical knowledge helps to treat common ailments. The main reason for associating plants with religious rites and beliefs is probably for conservation of rare plants which are under great threat of extinction.

Key words: alternative healthcare system; conservation; culture and tradition; environmental protection; ethnobotanical knowledge; hakims; sacred plants.

Introduction:

Plants occupy an important place in Indian mythology. Every nation has its own set of sacred plants. India is famous for its religious culture and traditions hence it is regarded as Veda Bhoomi, Punya Bhoomi, Karma Bhoomi (Land of Gods). Indian mythology records a plant as kalpavriksa, i.e a tree fulfilling all human desires. Since Vedic times, plants are considered as an indispensable source of both preventive and curative medicine. The World Health Organization estimated that 80% of the population of developing countries relies on traditional medicines, mostly plant drugs, for their primary health care needs. Different trees like neem (*Azadirachta indica*), banyan (*Ficus bengalensis*), bel (*Aegle marmelos*) and many more have been added to the religious sanctity. Even various Gods and Goddesses have been associated with different trees like bel, rudraksha (*Elaeocarpus sphaericus*) seeds are close to Lord Shiva, peepal to Lord Vishnu, mango (*Mangifera indica*) to Lord Hanuman etc. Our ancestors recorded some very important plants as sacred, which have enormous medicinal value.

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Research Article

Virtual screening, optimization of lead molecule selective inhibitors of farnesyl-protein transferase

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ABSTRACT

Farnesylation of the *ras* oncogene product by farnesyltransferase (FTase) is known to be a critical step in cell transformation leading to uncontrolled proliferation. Inhibitors of farnesyl-protein transferase (FPTase) have the potential of being anticancer agents for tumors in which *ras* was found mutated and contributes to cell transformation. As a result of the studies described herein, highly potent FPT inhibitors (FPTIs) with improved pharmacokinetic profiles have been identified. The post-translational addition of a farnesyl moiety to the Ras oncoprotein is essential for its membrane localization and is required for both its biological activity and ability to induce malignant transformation. We have prepared a series of potent ligand, inhibitors of the FPTase. The compounds were found to possess potent activity against enzymes. Mechanistic analysis had shown that the compounds are CAAX ("C" is cysteine, "a" is an aliphatic amino acid, and "X" is variable) competitive for FPTase inhibition. Then, compounds which passed ADMET (or) TOPKAT test were screened out. Based on the lowest energy, non-toxic molecules were docked with the FPTase receptor protein. Binding energy and docking results were observed for the comparative study of a good inhibitor against FPTase protein. The best molecule identified was further evaluated by molecular dynamics simulation of the protein-ligand complex. From the docking studies ligand, 1-[5-*tert*-butyl-2-(pyrazin-2-ylmethyl) phenyl]-2, 2-di hydroxy propan-1-one is the best ligand which can inhibit the target FPTase.

KEY WORDS: ADMET, CAAX, Cancer, Docking, Farnesyl-protein transferase, Farnesyl-protein transferase inhibitor, Phamacophore, Ras, Toxicity

INTRODUCTION

Cancer is a disease of uncontrolled cell growth in tissues. This growth may lead to metastasis, which is the invasion of adjacent tissue and infiltration beyond the site of initiation. Cancer is initiated by activation of oncogenes (or) inactivation of tumor suppressor genes. Mutations in the *K-ras* proto-oncogene are responsible for 10–30% of adenocarcinomas.

Ras gene mutations have been identified in approximately 30% of human cancers,[1-5] and evidence has prompted considerable efforts to elucidate the pathways of Ras transformations.

The key role of Ras proteins is cell growth and cell proliferation.[6] Ras proteins (H-Ras, K-Ras4A, K-Ras4B, and N-Ras) are small G-proteins which have the crucial role of transducing intracellular signals from growth factor receptor to several signal transduction pathways, such as the MAP-kinases cascade and the PI3-K/Akt pathway.[3,7-9] Activation of these signal transduction pathways by Ras is critical for cell growth, proliferation, and survival. Ras proteins require localization at the plasma membrane to exert their functions.

Membrane-bound GTP binding proteins (G-proteins) act as molecular switches to regulate cell growth by cycling between the inactive GDP- and the active GTP-bound state. In tumor cells, the constitutive activation of some G-proteins contributes to their malignant growth properties.[10] In normal cells, this switching mechanism is highly regulated, and G-proteins are found predominantly in their inactive GDP-binding state. All of these G-proteins originally have the CAAX tetrapeptide motif (C: Cys, A: an aliphatic amino acid, and X: Ser, Met, Gln, Ala) at their C-terminal.[11a-e] Farnesyltransferase (FTase) enzymes recognize this CAAX tetrapeptide motif and transfer the farnesyl group to the cysteine thiol. This farnesylation is critical for membrane binding and the biological function of G-proteins.[12]

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Apart from Ras, other proteins including RhoB, CENP-E, and CENP-F are also farnesylated and are also involved in mediating cell growth.[13,14a-f] Inhibition of the enzyme that catalyzes the farnesylation of Ras and farnesyl protein transferase (FPTase) leads to inhibition of tumor cell growth in *vitro* and *in vivo*.[15a-e]

Many classes of farnesyltransferase inhibitors (FTIs) have been reviewed.[8,16-20] In addition, the crystal structure of FTase was determined at 2.25 Å resolution and revealed essential information about the active site.[21] The existence of a high-affinity hydrophobic aromatic pocket[22,23] in the peptidic strategy based on the C-terminal CAAX motif of the Ras protein is the subject of increasing interest.

Human cancers resulted in a growing interest in FPT as a target for novel anti-cancer agents.[2,24] FPT not only plays a key role in enabling the Ras protein to acquire full biological activity as a signal transducer[3] but its substrates also include several other proteins which are critical intermediates of cell signaling and cytoskeleton organization.[4,16]

The authors have already published 1 research paper,[25] and 2 research papers are in print.[26,27]

MATERIALS AND METHODS

Ligand-based drug design is an iterative process with drug and virtual screening to score the biological activity of chemical molecules from the database. The molecules which give the best docking score are selected.

The model of the biological target may be built based on the knowledge of what binds to it through modeler. Quality of structure is then evaluated. One of the most important steps in drug design is structure analysis of protein active site. Ligand-based design methods capitalize on the fact that ligands similar to an active ligand are more likely to be active than random ligands.

Ligand-based quantitative structure-activity relationship approaches require a number of active molecules spanning a wide range of activity against the target. As high score compound is found, bioactivity

Table 1: A set of designed compound displaying and their molecular properties and ADMET properties

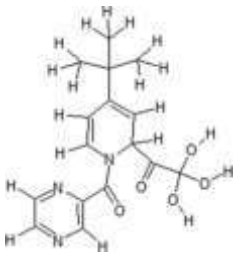
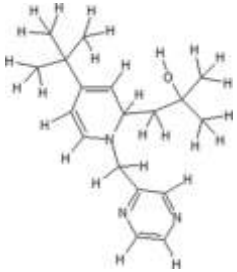
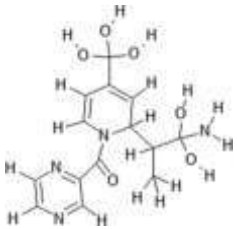
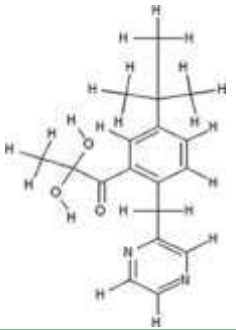
Drug molecule	A Log P	MW	Number of H acceptor	Number of H-Donar	Number of rotatable bonds	Number of rings	Number of aromatic rings	Molecular fractional surface area
1	0.069	333.339	7	3	4	2	1	0.362
2	1.533	301.426	4	1	5	2	1	0.145
3	−1.802	338.316	9	6	4	2	1	0.517
4	1.791	314.379	5	2	5	2	2	0.247
5	−2.946	290.278	8	3	3	2	1	0.502
6	−0.736	288.262	9	4	4	2	2	0.584
7	−2.538	295.294	8	3	3	2	1	0.476
8	−1.38	309.708	7	2	3	2	1	0.407
9	−1.006	273.247	6	1	3	2	1	0.435
10	−2.675	302.242	9	3	5	2	2	0.531
11	−0.372	279.184	8	1	4	2	1	0.521
12	−2.832	277.236	7	1	3	2	0	0.466
13	−2.756	275.263	6	3	3	2	1	0.492
14	0.338	320.276	8	4	5	2	2	0.49

Table 2: Toxicity prediction such as NTP and FDA carcinogenicity, rat oral LD_{50} and LC_{50} properties of designed drug molecule

Drug molecule	NTP carcinogenicity call (male rat) (v3.2)	DTP (v3.1)	Rat oral LD_{50} (v3.1)	Chronic LOAEL (v3.1)	Skin irritation (v6.1)	Aerobic biodegradability (v6.1)	NTP carcinogenicity call (female mouse) v3.2)
01	0.025	0.139	1.121	4.917	0.000	0.033	1.000
02	0.000	0.998	1.929	3.828	0.000	0.011	1.000
03	0.000	0.989	1.101	0.918	0.000	1.000	1.000
04	0.000	1.000	1.232	5.642	0.000	0.000	1.000
05	0.007	0.994	1.067	4.690	0.000	0.006	1.000
06	0.473	0.010	2.099	5.466	0.000	0.000	1.000
07	0.002	0.996	0.711	5.176	0.000	1.000	1.000
08	0.001	0.000	0.829	4.760	0.000	0.000	1.000
09	0.006	0.975	3.346	3.621	0.000	0.999	1.000
10	0.000	0.944	3.124	4.012	0.126	0.000	1.000
11	0.003	0.021	2.473	4.014	1.000	0.004	0.032
12	0.455	0.001	1.192	4.559	0.000	0.000	0.610
13	0.000	1.000	3.247	3.804	0.000	0.000	1.000
14	0.546	0.075	3.070	5.457	0.000	0.995	1.000

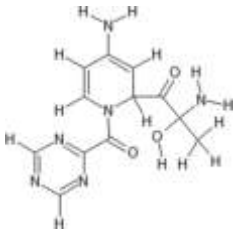
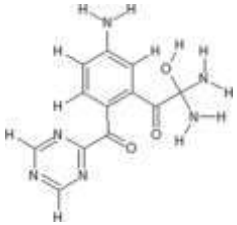
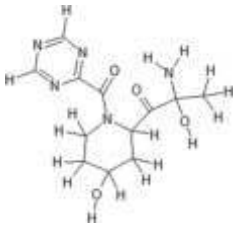
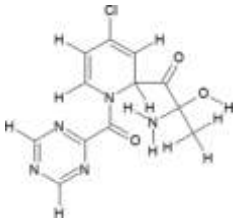
DTP: Developmental toxicity potential

Table 3: The list of 14 inhibitors with their C-Docker interaction energy to active site of FPTase

Drug molecule	Name of the molecule	Structure of the molecule	Docking energy (K.cal/mole)	Docking interaction energy (K.cal/mole)
01	1-[(2*R*)-4-*tert*-butyl-1-(pyrazin-2-yl carbonyl)-1,2-dihydr opyridin-2-yl]-2,2,2-trihydroxy ethanone		−325.687	−86.0551
02	1-[(2*R*)-4-*tert*-butyl-1-(pyrazin-2-yl methyl)-1,2-dihydro pyridin-2-yl]-2-methyl propan-2-ol		−375.595	−88.0314
03	[(2*S*)-2-[(2*S*)-1-amino-1,1-dihydroxypropan-2-yl]-4-(trihydroxymethyl) pyridin-1 (2*H*)-yl](pyrazin-2-yl) methanone		−510.163	−100.012
04	1-[5-*tert*-butyl-2-(pyrazin-2-ylmethyl) phenyl]-2,2-dihydro xypropan-1-one		−949.206	−140.796

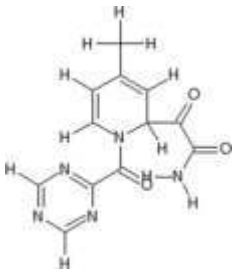
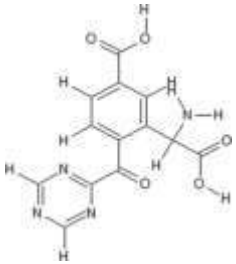
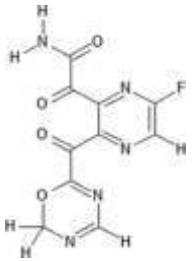
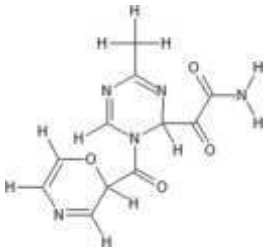
(*Contd...*)

Table 3: (Continued)

Drug molecule	Name of the molecule	Structure of the molecule	Docking energy (K.cal/mole)	Docking interaction energy (K.cal/mole)
05	(2S)-2-amino-1-[(2*S*)-4-amino-1-(1,3,5-triazin-2-ylcarbonyl)-1,2-dihydropyridin-2-yl]-2-hydroxy propan-1-one		−120.449	−25.6565
06	2,2-diamino-1-[5-amino-2-(1,3,5-triazin-2-ylcarbonyl) phenyl] -2-hydroxy ethanone		−138.302	−46.5741
07	(2*S*)-2-amino-2-hydroxy-1-[(2*S*,4*R*)-4-hydroxy-1-(1,3,5-triazin-2-ylcarbonyl) piperidin-2-yl] propan-1-one		−139.611	−29.5144
08	(2*S*)-2-amino-1-[(2*S*)-4-chloro-1-(1,3,5-triazin-2-ylcarbonyl)-1,2-dihydropyridin-2-yl]-2-hydroxypropan-1-one		−129.566	−28.9825

(*Contd...*)

Table 3: (Continued)

Drug molecule	Name of the molecule	Structure of the molecule	Docking energy (K.cal/mole)	Docking interaction energy (K.cal/mole)
09	2-[(2*S*)-4-methyl-1-(1,3,5-triazin-2-ylcarbonyl)-1,2-dihydropyridin -2-yl]-2-oxoacetamide		−123.453	−36.6684
10	3-[(*S*)-amino (carboxy) methyl]-4-(1,3,5-triazin-2-ylcarbonyl) benzoic acid		−106.821	−39.7161
11	2-[6-fluoro-3-(2*H*-1,3,5-oxadiazin-6-ylcarbonyl) pyrazin -2-yl]-2-oxoacetamide		−89.7994	-20.0638
12	2-{(2*R*)-4-methyl-1-[(2*S*)-2*H*-1,4-oxazin-2-ylcarbonyl]-1,2-dihydro -1,3,5-triazin-2-yl}-2- xoacetamide		−84.726	−18.4436

(*Contd...*)

Table 3: (Continued)

Drug molecule	Name of the molecule	Structure of the molecule	Docking energy (K.cal/mole)	Docking interaction energy (K.cal/mole)
13	(2*S*)-2-amino-2-[(2*S*)-4-hydroxy-1-(pyrazin-2-ylcarbonyl)-1,2-dihydropyridin-2-yl] ethanamide		−144.986	−15.1774
14	2-amino-1-{2-[(5-aminopyrazin-2-yl) carbonyl]-5-(fluoro methyl) phenyl}-2,2-dihydroxyethanone		−239.079	−78.4777

of these molecule should be tested on protein. Test is repeated a number of times to identify more ligand molecule improve the efficiency of previous ligand.

Drug library

Drug library is designed with the help of ACD-Chemsketch Software. A training set of compounds with inhibitory activities to FPTase enzyme was used to formulate the pharmacophore. Inhibition hypotheses that were subsequently used to examine ligand obtained from the docking studies.

Molecular modeling

Ligand-based drug design (or indirect drug design) relies on knowledge of other molecules that bind to the biological target of interest. A model of the biological target may be built based on the knowledge of what binds to it, and this model in turn may be used to design new molecular entities that interact with the target. Molecular modeling has been done by MODELLER 9v7, and design model gives hundred percent match to the protein. Therefore, we took this protein data banking (PDB id) for further analysis.

Docking

Molecular docking has become an indispensable part of structure-based drug designing in the past decades. In the most general since, docking is the prediction of optimal energy and spatial configuration between molecules. Therefore, by docking, the optimum configurations that maximize the interaction between protein and drug are searched. Discovery Studio v2.5 makes it easier to examine the properties of large and small molecules, study systems, identify leads, and optimize candidates.

Pharmacophore generation

The pharmacophore modeling approach utilizing the program catalyst was applied successfully to several problems in medicinal chemistry. Model building of characteristic chemical features of different inhibitors is critical task in drug discovery process and has turned into a particular useful application for the application for the virtual screening of large databases.

The level of finding active site is by pharmacophore studies. This is done using the tool LigandScout. This tool clearly picturizes the active site present hydrogen bond donor, hydrogen bond acceptor, negative and positive ionizable area, hydrophobic interaction, aromatic ring, and metal binding feature.

Tools and databases

NCBI, Swiss-port, Uniprot, Gene card databases were used for receptor identification and validation. FPTase structure was obtained from PDB database. Molecular modeling has been done using modeler 9v7 tool. Pharmacophore generation was done in Ligandscout.

Accelerys discovery studio was used for active site prediction to particular receptor, molecular dynamic simulation. Docking simulation was done in C-Docker tool of discovery studio and ADMET (absorption, distribution, metabolism, and excretion - toxicity in pharmacokinetics) tools used for toxicity prediction.

RESULTS AND DISCUSSION

Initially, 29 compounds were built and minimized to allow the docking in the crystal structure of human FPTase were tested for their ability to inhibit FPTase activity.

The modeling program discovery studio provides a reasonable explanation for the inhibitory activity of these compounds. The docking revealed an additional interaction between scaffolds constitutes an interesting pattern to position in the groups at the binding site of the FPTase pocket, this hydrophobic pocket has often been referred to as an important element for enzyme-inhibitor recognition.

Selection of hit molecules is based on either geometrical constraints or interaction energies between protein and ligand. The active site favours the binding of Ligand with the receptor. The 3D conformations docking interaction among the 14 ligand studies conclude only one best interaction energies between ligand and protein at the active site. The binding mode could explain the FPTase inhibitor activity best among the ligand. Figure 1 displays the proposed binding mode into the active site of FTase, confirming the good fit of the ligand into the binding site of the enzyme. Ligand is binded with LYS 164 A amino acid at the binding site of the enzyme. The docking energy and docking interactive energy of 1-[5-*tert*-butyl-2-(pyrazin-2-ylmethyl)phenyl]-2,2-dihydroxypropan-1-one is -949.26 and -140.796 K.cal/Mole. Among these 14 Drug molecules, 1-[5-tert-butyl-2-(pyrazin-2-ylmethyl) phenyl]-2,2-dihydro xypropan-1-one has the potent drug, which has capacity to bind with the Binding site. It inhibits the function of FPTase. (Figures 2-4).

These results suggest the molecular basis of FPTase inhibition by ligand 1-[5-*tert*-butyl-2-(pyrazin-2-ylmethyl) phenyl]-2, 2-dihydroxypropan-1-one. In particular, this compound inhibits the FTase selectively occupying the binding site of corresponding to the C-terminal sequence of the p21 Ras protein.

Result of clustal distance matrix is shown in Figure 5.

From Figure 3, sequence analysis shows that farnesyl protein showed maximum identities with *Mus musculus* (80%) and *Rattus novegicus*. Structure analysis shows that farnesyl protein is unstable and hydrophilic in nature. Farnesyl protein also shows much interaction with other body proteins

CONCLUSION

Our study describes the pharmacological evaluation of a series of compounds derived hydrophobic interaction with the FPTase binding site. From a consideration

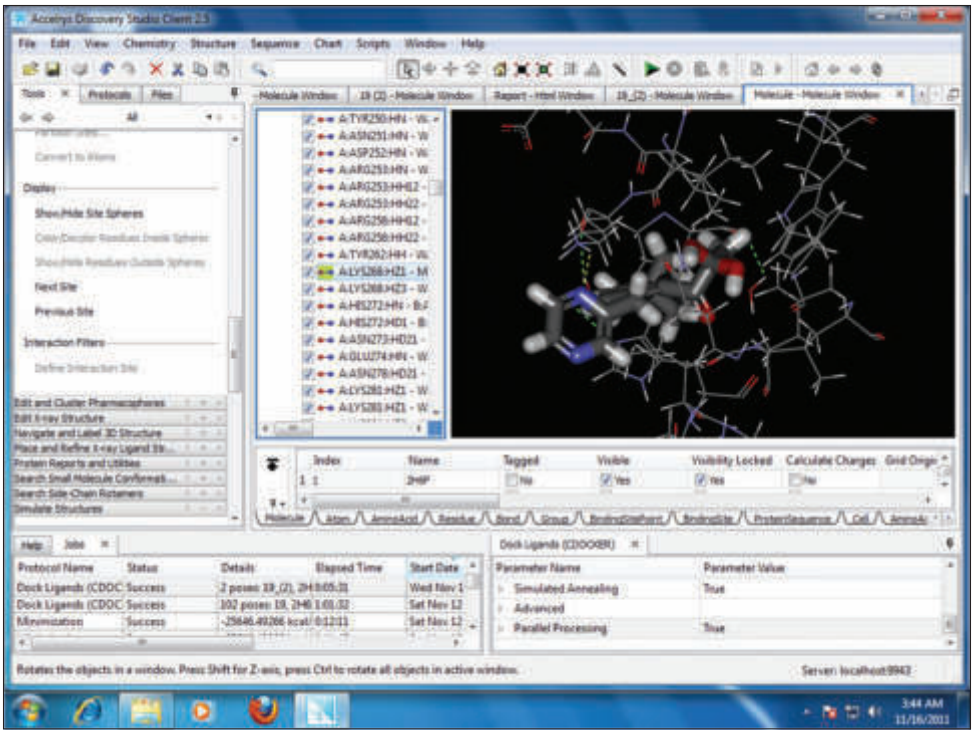


Figure 1: Binding orientation of designed compound (1-[5-*tert*-butyl-2-(pyrazin-2-ylmethyl)phenyl]-2,2-dihydroxypropan-1-one with FPTase enzyme active site. Colors observed in discovery studio N atom - blue color, colorless - C-H bonds

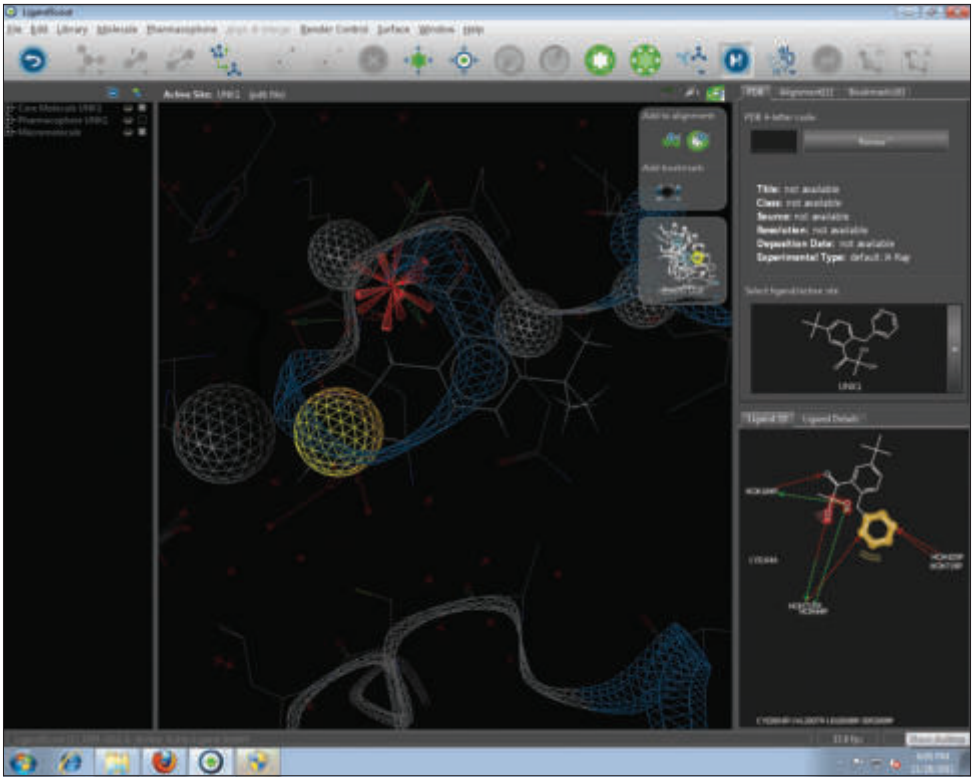


Figure 2: Binding orientation of designed compound (1-[5-*tert*-butyl-2-(pyrazin-2-ylmethyl) phenyl]-2,2-dihydroxypropan-1-one with FPTase enzyme active site. This figure shows effected area due to binding of ligand. Aromatic ring features (yellow), hydrophobic region feature (blue), hydrogen bond acceptor feature (red), hydrogen bond donor (green)

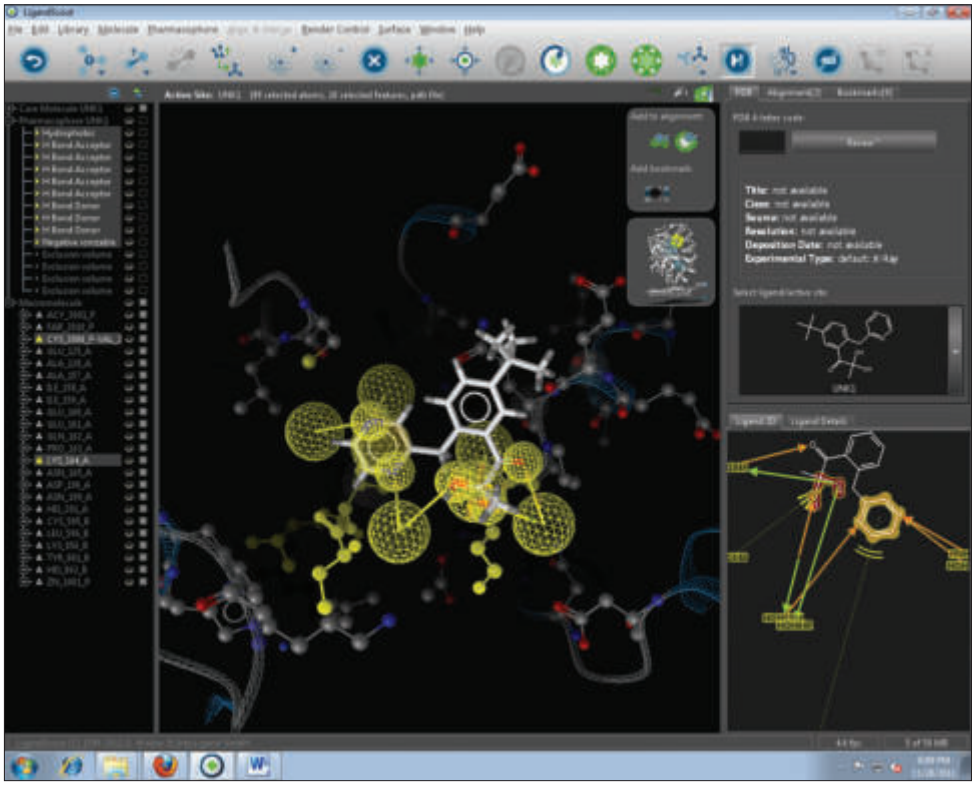


Figure 3: Binding orientation of designed compound (1-[5-*tert*-butyl-2-(pyrazin-2-ylmethyl)phenyl]-2,2-dihydroxypropan-1-one with FPTase enzyme active site. This figure shows H-bonding due to binding of ligand. Aromatic ring features (yellow), hydrophobic region feature (blue), hydrogen bond acceptor feature (red), hydrogen bond donor (green)

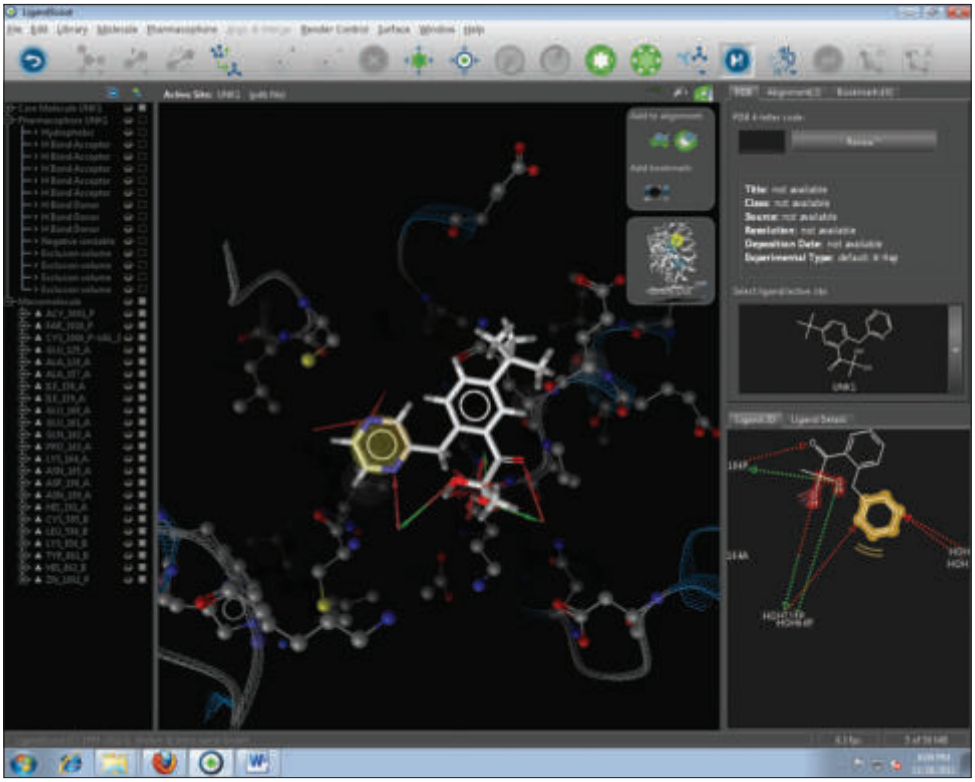


Figure 4: The designed compound with binding pocket of FPTase overlaid on four features of pharmacophore model. Aromatic ring features (yellow), hydrophobic region feature (blue), hydrogen bond acceptor feature (red), hydrogen bond donor (green)

of all parameters and their binding interaction with receptor binding site, work by blocking an enzyme, pharmacophore of regarding drug molecule was generated in the ligand.

Based on binding energy and hydrogen bond formed, docking results conclude that the ligand 1-[5-*tert*-butyl-2-(pyrazin-2-ylmethyl) phenyl]-2,2-dihydroxypropan-1-one is the best ligand which inhibits the target FPTase.

From our analysis, the 1-[5-*tert*-butyl-2-(pyrazin-2-ylmethyl) phenyl]-2,2-dihydroxypropan-1-one is the potent inhibitor. The ligand binds with LYS 168 amino acid at the binding site.

Figures 2-4 show the binding orientation of designed compound (1-[5-*tert*-butyl-2-(pyrazin-2-ylmethyl) phenyl]-2, 2- dihydroxypropan-1-one with FPTase enzyme active site. Figure 2 shows the designed compound with binding pocket of FPTase overlaid on four feature of pharmacophore- model. From ADMET properties (Table 1) molecular properties, toxicity properties (Table 2), docking score (Table 3).

Table 1 gives the ADMET properties of 14 ligand molecules gives the interaction with the binding site of the receptor. Among these drug molecule, 1-[5-tert-butyl-2-(pyrazin-2-ylmethyl) phenyl]-2,2-dihydro xypropan-1-one is potent drug, which binds with the Binding site.

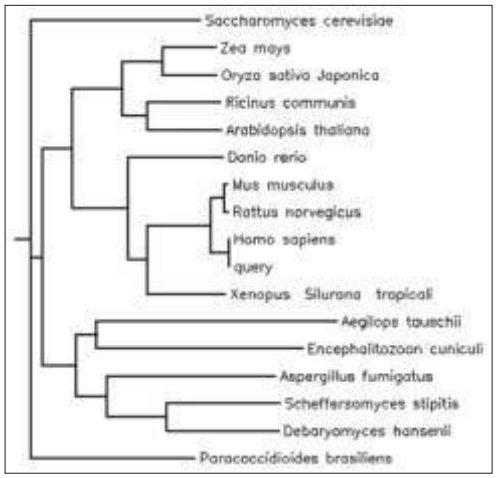


Figure 5: Clustal distance matrix result

Table 2 shows the toxicity prediction of designed 14 drug molecules. Among these ligands, ligand molecule number 4 shows more toxic property compared to the remaining drug molecules.

Table 3 shows the list of 14 inhibitors showing C Docker interaction energy to the active site of FPTase (−949.26), and C-Docker interaction energy (−140.796) of ligand to receptor binding site show that this drug molecule could be the best inhibitor toward FPTase.

These studies carried out that on the most potent ligand 1-[5-*tert*-butyl-2-(pyrazin-2-ylmethyl) phenyl]-2, 2-dihydroxypropan-1-one is the FTase inhibitor of the binding site, of which corresponds to the *C*-terminal sequence of p21 Ras protein.

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RISK MANAGEMENT IN BANKING SECTOR: EMERGING ISSUES AND TRENDS

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Abstract

Since the financial crisis, banks have gotten smarter about the way they manage their risks. It is no surprise that risk management in banks is changing and the risks involved are rising. Increased global competition, changing regulatory requirements, increased digitalisation and advances in technology are challenging the way banks interact with clients. There is also competition in the form of non bank firms expanding into the banking industry who want to take over the direct customer relationship and tap into the most lucrative part of the value chain—origination and sales. In this paper an attempt has been made to study the importance of risk management in banks and to review the emerging trends and issues in risk management in the banking sector.

Keywords: Bad Loans, Basel Accords, Cashless economy, Fintech , Risk Management

I INTRODUCTION

Banks have traveled a hard road since the global financial crash of 2008. They find themselves to be continually exposed to a variety of risks driven by the economic, geopolitical, technological, sociopolitical and environmental factors. While the magnitude and speed of regulatory change is unlikely to be uniform across countries, the future undoubtedly holds more regulation—both financial and non-financial—even for banks operating in emerging economies [1].

Largely in response to regulations that emerged from the 2008 crisis, risk management in banking has transformed over the past decade. Important trends are afoot that suggests risk management will experience even more sweeping changes in the next decade [2]. So unless banks are prepared to be proactive they will be left behind. Organisations must look at and be prepared for the continuum of risks that encompass not only known and unknown risks, but also those that are 'unknowable' or that require elements of 'black swan' management [1].

II OBJECTIVES

This study mainly intends to examine the following objectives.

- To study the importance of risk management in banks
- To study the emerging trends and issues in Bank risk management especially in the context of India.

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Synthesis and Antimicrobial Activity of 3-(1-Aryl-1*H*-1,2,3-triazol-4-yl)-2-(4-fluorophenyl)-1-(2-hydroxy-4-methoxyphenyl)propan-1-ones[1]

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Abstract—A number of novel 3-(1-aryl-1*H*-1,2,3-triazol-4-yl)-2-(4-fluorophenyl)-1-(2-hydroxy-4-methoxyphenyl)propan-1-ones has been synthesized from 2-(4-fluorophenyl)-1-(2-hydroxy-4-methoxyphenyl)ethanone by its propargylation followed by the click reaction. Structures of all the newly synthesized compounds were characterized by ^{1}H and ^{13}C NMR, and Mass spectra. Their antimicrobial activity was evaluated.

Keywords: fluorinated organic molecule, propargylation, click reaction, 1,2,3-triazole, antimicrobial activity

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INTRODUCTION

Fluorinated compounds are highly lipophilic which allows their molecules to be easily delivered to the active sites across the living body. Since there is only a limited number of naturally occurring fluorine-containing compounds, there is a certain demand in developing synthetic approaches to fluorinated organic compounds with biological potential. 1,2,3-Triazole and its derivatives demonstrate diverse biological activities such as antimicrobial [1], antiproliferative [2], antibacterial [3], anti-HIV [4], antifungal [5], anticancer [6], and antitubercular [7]. Based on the above, we have synthesized 3-(1-aryl-1*H*-1,2,3-triazol-4-yl)-2-(4-fluorophenyl)-1-(2-hydroxy-4-methoxyphenyl)propan-1-ones (Scheme 1).

RESULTS AND DISCUSSION

A number of novel 3-(1-aryl-1*H*-1,2,3-triazol-4-yl)-2-(4-fluorophenyl)-1-(2-hydroxy-4-methoxyphenyl)-propan-1-ones (**3a**–**3h**) has been synthesized from 2-(4-fluorophenyl)-1-(2-hydroxy-4-methoxyphenyl)ethanone (**1**) by its propargylation in the presence of K_2CO_3 in dry acetone to afford 2-(4-fluorophenyl)-1-(2-hydroxy-4-methoxyphenyl)pent-4-yn-1-one (**2**). Upon treatment of the compound **2** by various aryl azides in the presence of $CuSO_4 \cdot 5H_2O$ and sodium ascorbate in *t*-BuOH–H_2O media the title compounds were accumulated with high yields.

Spectral analysis, ^{1}H and ^{13}C NMR, and mass spectra, supported the structures of all synthesised compounds.

Antimicrobial activity. All synthesized compounds were screened for antibacterial activity against five gram positive and five gram negative bacterial strains: *M. Tuberculosis, M. Luteus, MRSA, B. Subtilis, B. Cereus, P. Aerginosa, K. Pneumonia, E. Coli, P. Vulgaris,* and *S. Typhi* using Gentamycin as a standard drug [8–10]. Among all compounds **3b** and **3d** demonstrated the highest activity against *K. Pneumonia* and *E. Coli*. The compounds **3a** and **3d** were most active against *K. pneumonia* and *E. coli.* The compounds **3a** and **3f** demonstrated the pronounced activity against *B. Subtilis* and *B. Cereus.*

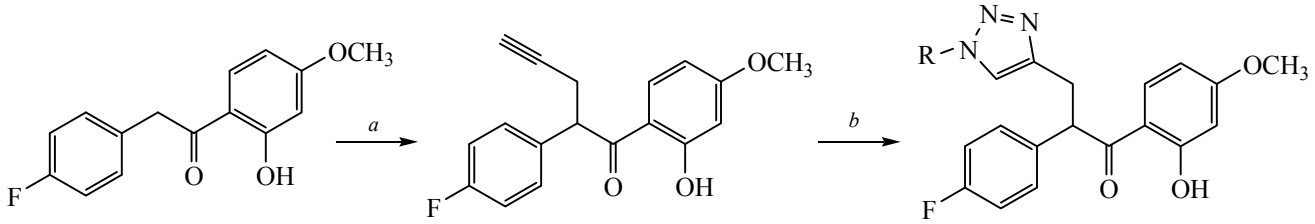
Antifungal activity. The synthesized compounds were also screened for antifungal activity against five fungal strains, including *T. Interdigitale, E. Floccosum, M. Canis, M. Gypseums,* and *Rubrum* using Nystatin as a standard drug [8–10]. The compound **3b** inhibited completely *M. Canis* and *M. Gypseums* and demonstrated the moderate activity against *T. Interdigitale*.

EXPERIMENTAL

Melting points were determined in open capillary tubes and are uncorrected. Purity of the compounds was tested by TLC using precoated silica gel plates 60_{254} (Merck). ^{1}H and ^{13}C NMR spectra were measured on a Bruker Avance II 400 MHz spectrometer using

[1] The text was submitted by the authors in English.

Scheme 1. Synthetic pathway to 3-(1-aryl-1*H*-1,2,3-triazol-4-yl)-2-(4-fluorophenyl)-1-(2-hydroxy-4-methoxyphenyl)propan-1-ones.



1 **2** **3a–3h**

a: propargyl bromide, K_2CO_3, dry acetone; *b:* R–N_3, $CuSO_4 \cdot 5H_2O$, sodium ascorbate, *t*-butanol, water.

TMS as an internal standard. Mass spectra were measured on a GCMS-QP 1000 EX mass spectrometer. Elemental analysis was carried out on a Thermo Finnigan CHNS analyzer.

Synthesis of 2-(4-fluorophenyl)-1-(2-hydroxy-4-methoxyphenyl)pent-4-yn-1-one (2). A mixture of 2-(4-fluorophenyl)-1-(2-hydroxy-4-methoxyphenyl)-ethanone (**1**) (1 mmol) with propargyl bromide (1.2 mmol) and potassium corbonate in dry acetone was refluxed for 8 h under TLC control. Upon completion of the process, the was mixture cooled down to room temperature and poured in ice cold water The precipitated solid was filtered off, washed with water and purified by column chromatography using ethyl acetate: heaxane as an eluent. Yield 55%, mp 164–166°C. ^{1}H NMR spectrum, δ, ppm: 1.94–1.96 t (1H, CH), 2.64–2.71 d.d (1H, CH_2), 2.94–3.01 d.d (1H, CH_2), 3.80 s (3H, OCH_3), 4.67–4.71 d.d (1H, CH), 6.35–6.40 m (2H, ArH), 6.99–7.03 m (2H, ArH), 7.28–7.31 m (2H, ArH), 7.61–7.63 d (1H, ArH), 12.68 s (1H, OH). ^{13}C NMR spectrum, δ_C, ppm: 29.7, 55.5, 61.6, 77.2, 101.0, 107.6, 108.0, 115.9, 116.1, 128.8, 129.5, 130.5, 132.2, 167.69, 189.4. MS 299 $[M - H]^+$.

Synthesis of 3-(1-Aryl-1*H*-1,2,3-triazol-4-yl)-2-(4-fluorophenyl)-1-(2-hydroxy-4-methoxyphenyl)-propan-1-ones (3a–3h). A mixture of 2-(4-fluorophenyl)-1-(2-hydroxy-4-methoxyphenyl)pent-4-yn-1-one (**2**) (1 mmol) with a certain azide (1 mmol), $CuSO_4 \cdot 5H_2O$ and sodium ascorbate in *t*-BuOH–H_2O (2 : 1) was stirred at room temperature until completion of the reaction according to TLC (15–20 h). Then it was poured into ice cold water. The precipitated solid was filtered off and purified by column chromatography using ethyl acetate: heaxane as an eluent.

2-(4-Fluorophenyl)-1-(2-hydroxy-4-methoxyphenyl)-3-(1-phenyl-1*H*-1,2,3-triazol-4-yl)propan-1-one (3a). Yield 84%, mp 180–182°C. ^{1}H NMR spectrum, δ, ppm: 3.18–3.24 d.d (1H, CH_2), 3.62–3.68 d.d (1H, CH_2), 3.76 s (3H, OCH_3), 5.11–5.15 d.d (1H, CH), 6.32–6.35 m (2H, ArH), 7.01–7.06 m (2H, ArH), 7.27–7.34 m (3H, ArH), 7.37–7.40 m (2H, ArH), 7.45–7.54 m (2H, ArH), 7.58–7.73 m (2H, ArH), 12.76 s (1H, OH). ^{13}C NMR spectrum, δ_C, ppm: 29.8, 51.6, 55.6, 66.6, 101.0, 107.8, 112.8, 115.9, 116.4, 120.2, 120.4, 128.6, 128.8, 129.5, 129.6, 129.7, 130.9, 132.0, 132.2, 134.8, 134.8, 136.9, 166.1, 166.2, 167.6, 202.7. MS 418 $[M - H]^+$.

3-[1-(2-Chlorophenyl)-1*H*-1,2,3-triazol-4-yl]-2-(4-fluorophenyl)-1-(2-hydroxy-4-methoxyphenyl)-propan-1-one (3b). Yield 77%, mp 202–204°C. ^{1}H NMR spectrum, δ, ppm: 3.24–3.29 d.d (1H, CH_2), 3.62–3.68 d.d (1H, CH_2), 3.78 s (3H, OCH_3), 5.08–5.12 d.d (1H, CH), 6.34–6.46 m (2H, ArH), 6.98–7.01 m (2H, ArH), 7.27–7.32 m (2H, ArH), 7.39–7.42 m (2H, ArH), 7.50–7.55 m (2H, ArH), 7.68–7.73 m (2H, ArH), 12.77 s (1H, OH). ^{13}C NMR spectrum, δ_C, ppm: 29.6, 51.6, 55.5, 61.6, 101.0, 107.8, 112.8, 115.8, 116.1, 127.6, 127.8, 128.8, 129.5, 129.6, 130.6, 130.9, 132.0, 132.2, 166.1, 166.2, 167.6, 202.7. MS 452 $[M - H]^+$.

3-[1-(3-Chlorophenyl)-1*H*-1,2,3-triazol-4-yl]-2-(4-fluorophenyl)-1-(2-hydroxy-4-methoxyphenyl)-propan-1-one (3c). Yield 80%, mp 191–193°C. ^{1}H NMR spectrum, δ, ppm: 3.17–3.22 d.d (1H, CH_2), 3.61–3.67 d.d (1H, CH_2), 3.75 s (3H, OCH_3), 5.12–5.19 d.d (1H, CH), 6.32–6.35 m (2H, ArH), 6.86–7.01 m (2H, ArH), 7.28–7.46 m (5H, ArH), 7.63–7.68 m (2H, ArH), 7.81–7.83 m (1H, ArH), 12.77 s (1H, OH). ^{13}C NMR spectrum, δ_C, ppm: 29.6, 51.6, 55.5, 61.6, 101.0, 107.8, 112.8, 115.8, 116.1, 127.6, 127.8, 128.8, 129.5, 129.6, 130.6, 130.9, 132.0, 132.2, 166.1, 166.2, 167.6, 202.7. MS 452 $[M - H]^+$.

2-(4-Fluorophenyl)-1-(2-hydroxy-4-methoxyphenyl)-3-[1-(*p*-tolyl)-1*H*-1,2,3-triazol-4-yl]propan-1-one (3d). Yield 86%, mp 175–177°C. ^{1}H NMR spectrum, δ, ppm: 1.85 s (1H, CH_3), 3.10–3.16 d.d (1H, CH_2), 3.45–3.51 d.d (1H, CH_2), 3.72 s (3H, OCH_3), 5.01–5.08 d.d (1H, CH), 6.33–6.35 m (2H, ArH), 6.82–6.88 m (2H, ArH), 7.13–7.20 m (2H,

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Antimicrobial Activity of Newly Synthesized and Characterized of Mixed Bi-Heterocyclic Azo Compound (3-Pyridyl-Azo-Benzimidazole)

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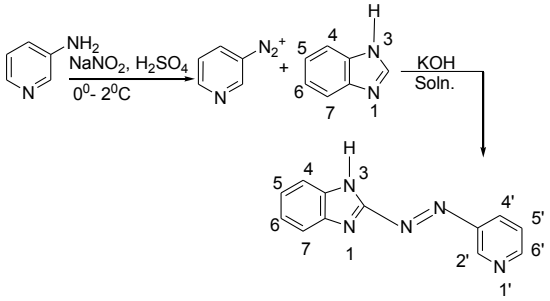
Azo-imine group containing Pyridine and benzimidazole bi-heterocyclic azo compound should have versatile activities in biological fields. We are convinced from the literature survey of pyridine and benzimidazole derivatives to synthesize pyridine and benzimidazole containing mixed bi-heterocyclic azo compound, (2-[(3-pyridyl)azo]benzimidazole). Synthesis has been carried out by the reaction between diazonium salt of 3-aminopyridine with the benzimidazole in alkaline solution at low temperature. The structure of the newly synthesized compound has been characterized on the basis of IR, UV-Vis, ^{1}H NMR and Elemental analysis. Investigation of invitro anti-microbial activity of synthesized compound was done by well diffusion method against some common Gram positive and Gram negative bacteria. The successfully synthesized compound exhibited highest to moderate inhibitory effect against Gram-negative bacteria Pseudomonas fluorescence, Salmonella sp and E. Coli.



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Microwave assisted synthesis and antimicrobial activity of 4-((4-substitutedphenyl)sulfonyl)morpholines

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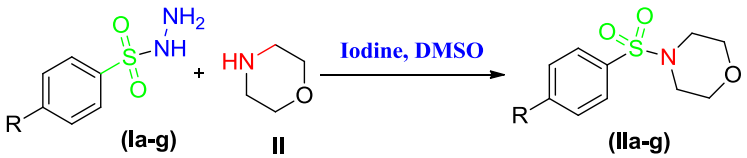
A series of 4-((4-Substitutedphenyl)sufonyl)morpholines have been synthesized from 4-substitutedbenzenesulfonohydrazides and morpholine under microwave irradiation and conventional heating methods. All the compounds tested for their in vitro antimicrobial activity against bacterial and fungal organisms and they were characterized on the basis of spectral data such as IR, ^{1}H NMR, ^{13}C NMR, mass spectral data and elemental analysis.



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ORIGINAL ARTICLE

Analysis of anti-bacterial and anti oxidative activity of *Azadirachta indica* bark using various solvents extracts

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KEYWORDS

Anti-bacterial activity;
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Azadirachta indica

Abstract Herbal medications have been used for relief of symptoms of disease. Regardless of the great advances observed in current medicine in recent decades, plants still make a significant contribution to health care. An alarming increase in bacterial strains resistant to a number of antimicrobial agents demands that a renewed effort be made to seek antibacterial agents effective against pathogenic bacteria resistant to or less sensitive to current antibiotics. Anti-bacterial activity of *Azadirachta indica* stem bark was tested against pathogenic *Salmonella paratyphi* and *Salmonella typhi* using various solvent extracts. The in vitro anti-bacterial activity was performed by agar well diffusion method and the results were expressed as the average diameter of zone of inhibition of bacterial growth around the well. The ethanol and methanol extracts showed better anti-bacterial activity with zone of inhibition (20–25 mm) when compared with other tested extracts and standard antibiotic Erythromycin (15 mcg) with zone of inhibition (13–14 mm). Using Fisher's exact test of significance difference was found between two Salmonella strains sensitivity patterns against tested extracts ($P \leqslant 0.035$). Extracts of *A. indica* stem bark also exhibited significant antioxidant activity, thus establishing the extracts as an antioxidant. The results obtained in this study give some scientific support to the *A. indica* stem bark for further investigation of compounds and in future could be used as drug.

1. Introduction

Herbal medications have been used for relief of symptoms of disease (Maqsood et al., 2010). Regardless of the great advances observed in current medicine in recent decades, plants still make a significant contribution to health care. Much interest, in medicinal plants however, emanates from

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Effect of sintering temperature on leakage current of polycrystalline multiferroic $DyFeO_3$ system

S. Shravan Kumar Reddy, N. Raju, J. Ramesh, Ch. Gopal Reddy, P. Yadagiri Reddy, K. Rama Reddy & V. Raghavendra Reddy

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^{57}Fe Mössbauer study of spin reorientation transition in polycrystalline $NdFeO_3$

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ABSTRACT

The present work reports the preparation of polycrystalline $NdFeO_3$ using sol-gel method and characterization using X-ray diffraction (XRD), Raman spectroscopy, bulk magnetization, ^{57}Fe Mössbauer spectroscopy and ferroelectric measurements. XRD and Raman spectroscopy measurements confirm the phase purity of the prepared sample. The temperature dependent magnetization measurement shows the signatures of spin re-orientation transition (T_{SRT}) between 66 and 158 K and magnetic field induced transition at about 2.5 T and 5 K. It is observed from the low temperature (25–300 K) ^{57}Fe Mössbauer measurements that the temperature variation of hyperfine parameters shows the signatures of T_{SRT}. The observed area ratio of second and third line intensity (A_{23}) in Mössbauer sextet, across T_{SRT}, show deviations from the value characteristic of random spin orientation in polycrystalline sample. In addition, the quadrupole shift changes sign across T_{SRT} indicating the spin-reorientation of Fe^{3+} ions. The room temperature leakage current density (*J-E*) measurements indicate that Ohmic contribution and space charge limited conduction are the dominating mechanisms at low and high applied electric fields, respectively, similar to that of other $RFeO_3$ (R – rare earth) based compounds. Lossy ferroelectric loops were observed at room temperature.

1. Introduction

The rare earth ortho-ferrites $RFeO_3$ (R-rare earth atoms) are studied extensively in recent literature in the context of discovery of magneto-electric (ME)/multiferroic nature [1]. These compounds exhibit an array of interesting magnetic properties/transitions, viz., paramagnetic to antiferromagnetic (AFM) ordering of Fe^{3+} ions (Neel transition (T_N)), spin-reorientation transition of Fe^{3+} ions (T_{SRT}) and magnetic ordering of rare-earth ions, compensation point etc, as result of interactions between two magnetic sublattices of iron and rare-earth viz., Fe^{3+} - Fe^{3+}, R^{3+}- Fe^{3+} and R^{3+}-R^{3+} magnetic exchange interactions [2,3]. The magneto-electric (ME) materials exhibit ferroelectric and magnetic ordering simultaneously and coupling between these two orders. Usually it is difficult to observe these two orders simultaneously, as the magnetism requires presence of electrons in the d-shells of the transition metal ions which prevent the occurrence of ferroelectric order [4]. Single crystal $DyFeO_3$ exhibits large ME coupling at about 4 K, which is explained in terms of exchange-striction between adjacent Fe^{3+} and Dy^{3+} layers with the respective layered antiferromagnetic (AFM) components [5]. Similarly the mutual controllability of both the magnetic and ferroelectric order parameters in single crystal $GdFeO_3$ is reported and explained the results in terms of exchange interaction between the Gd and Fe spins [6]. Aparnadevi et al. have reported multifunctional properties in polycrystalline $NdFeO_3$ prepared by ball-milling method. The coupling between magnetic and electric order parameters are demonstrated with dielectric impedance spectroscopy measured as a function of external magnetic field [7]. $NdFeO_3$ exhibits weak antiferromagnetism, similar to that of other $RFeO_3$ compounds, of G-type with T_N at about 697 K and spin reorientation (T_{SRT}) phenomenon between 70 K and 160 K [8].

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Study of Mn doped multiferroic $DyFeO_3$ ceramics

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ABSTRACT

Structural, Raman, room temperature and temperature dependent leakage current density, dielectric, magnetization and room temperature Mossbauer studies of Mn doped $DyFeO_3$ (i.e., $DyFe_{1-x}Mn_xO_3$; x=0 to 0.5) polycrystalline materials prepared through sol-gel route are reported in this paper. From Rietveld refinement of x-ray diffraction (XRD) patterns it is found that all the samples are formed in single phase without any detectable impurity. The Raman modes with doping are consistent with literature of such doped orthoferrites. From the room temperature (RT) leakage current density (J-E) measurements, it is observed that leakage current density increases with Mn doping concentration, which is explained in terms of microstructure. The leakage current density is found to decrease with the decrease of temperature in each sample as observed from low temperature leakage current density (J-E) measurements. Further, activation energy is calculated from the temperature dependent J-E data. The dielectric loss data is observed to exhibit frequency dependence and the activation energy obtained indicate the contribution from space charges. From temperature dependent magnetization data, it is found that with the increase of Mn content, the spin reorientation (SR) transition temperature (T_{SR}) moves towards higher temperature. From M-H curves at 10 K and 300 K with different Mn doping concentrations, it is found that saturation Magnetization (M_S) decreases with increase of Mn doping. Room temperature Mossbauer data shows the presence of Fe^{3+} state and the gradual decrease of internal hyperfine filed with increase of Mn content.

1. Introduction

In the recent years, multiferroic/magneto-electric (ME) materials research has increased interest in the scientific community and becoming emerging field, as they are promising candidates for technical applications in various fields and rich physics involved [1–3]. Magneto-electric (ME) materials exhibit simultaneous ferroelectric and magnetic ordering, although it is difficult to observe these two orderings simultaneously, as the magnetism requires presence of electrons in the d-shells of the transition metal ions which prevent the occurrence of ferroelectric ordering. However many materials, specifically oxide materials such as rare earth manganites ($RMnO_3$), rare earth chromites ($RCrO_3$), rare earth orthoferrites ($RFeO_3$), RMn_2O_5 and RFe_2O_4 are reported as multiferroic/ME materials with different origins of ferroelectricity [4–6]. Among all of them, rare-earth orthoferrites of general formula $RFeO_3$ (R=Rare earth) are a special class of materials exhibiting large ME coupling. $DyFeO_3$ is a rare-earth ortho-ferrite of $RFeO_3$ (R=Dy, Rare-earth) group. This material is recently reported to exhibit large ME coupling at about 4 K and magnetic field induced ferroelectricity in single crystal $DyFeO_3$ [7], which was explained in terms of exchange-striction between adjacent Fe^{3+} and Dy^{3+} layers with the respective layered antiferromagnetic (AFM) components. $DyFeO_3$ crystallizes in orthorhombic distorted (ABO_3) perovskite structure with centro-symmetric space group Pbnm. $DyFeO_3$ exhibits Fe^{3+}-Fe^{3+}, Dy^{3+}-Fe^{3+} and Dy^{3+}-Dy^{3+} exchange interactions. Due to these interactions, $DyFeO_3$ exhibits spin reorientation of Fe^{3+} spins from canted AFM to collinear AFM state. It is reported that substitution of Mn^{3+} ions at Fe-site increases spin reorientation transition temperature (T_{SR}) and decreases Neel temperature (T_N) [8,9]. Substitution of about 40% Mn at Fe site results these two temperatures to be close to room temperature [9] and therefore has been argued to be the suitable material from the room temperature application point of view. However, most of the previous studies on $DyFe_{1-x}Mn_xO_3$ system were discussed only based on magnetization measurements [8,9]. ^{57}Fe Mossbauer measurements give the microscopic information about the magnetic ordering present, valence of Fe

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Classification of DNA Sequence Using Soft Computing Techniques: A Survey

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Abstract

Objectives: This survey detects which methodology of soft computing are used frequently together to solve the problems of Deoxyribonucleic acid (DNA) sequencing and provides an overview of underlying concepts commonly used for DNA classification using soft computing technique. **Methods/Analysis:** DNA sequence classification is a significant problem in computational biology. The DNA sequence is used to identify differences and similarities between organisms within a species. The selection of attributes is primary criteria in DNA classification. DNA sequence classification techniques involve for origin of particular characteristics from the progressions. Different species have distinct genetic structure. **Findings:** The distinctive asset of soft computing is that helps to learn from empirical procedure that helps for DNA classification. The major components of Soft Computing are Fuzzy Sets (FS), Artificial Neural Networks (ANN), Genetic algorithms (GAs), Evolutionary Strategies (ES), Support Vector Machines (SVM), Rough Sets (RS), Simulated Annealing (SA), biological inspired Swarm Optimization (SO), Ant Colony Optimization (ACO) and Tabu Search (TS). Soft Computing techniques are recognized as gorgeous options to the standard, conventional hard computing methods. **Novelty /Improvement:** This paper presents to identify the DNA sequences using the different classification approaches have been proposed by various researchers.

Keywords: Classification, DNA Sequence, Soft Computing techniques

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CLASSIFICATION OF DNA BARCODES BASED ON IMAGE PROCESSING TECHNIQUES: A STUDY

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ABSTRACT

DNA barcoding is a method of identifying the species in biological scientific community without involving the morphological clues. DNA barcoding is a molecular method and which uses DNA from a standardized region of the genome to identify the species. Barcodes are machine readable and capable of storing digital information. The image processing based barcode reading systems started to gain importance which provide more information than laser barcode readers at a time. In this paper, a few traditional barcode methods, computer vision based decoding techniques, image processing based barcode reading system & methods and its performance issues are discussed. Image processing based barcode recognition systems are expected to increase the performance in barcode reading. Preprocessing, segmentation, edge detection and optimization techniques were used in DNA barcode classification.

KEYWORDS: DNA barcode, Barcode recognition systems, Decoding techniques, Segmentation and Edge detection

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Oxidation of Glycylglycine by $KBrO_3$ in Aqueous Acetic Acid Medium and Comparison with Monomer Glycine: A Kinetic and Mechanistic Study

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The kinetics of oxidation reactions of dipeptide glycylglycine (GG) by $KBrO_3$ in aqueous acetic acid medium, under the condition $[KBrO_3] << [GG]$ at different temperatures (313-323 K), to produce formic acid, ammonia, carbon dioxide and water were studied. Study of the kinetic results showed that the first order dependence in $[KBrO_3]$ and fractional order dependence in [GG]. The effect of ionic strength and [AcOH] on rate was studied and thermodynamic parameters were also calculated. Michealis-Menten type mechanism was proposed.

Keywords: Glycylglycine, Glycine, Potassium bromate, Acetic acid.

INTRODUCTION

Bromate is a hypervalent oxyanion of bromine, which is known as a versatile oxidizing agent [1-5] and brominating agent depending on reaction conditions. It oxidizes reducing agents and can be reduced to bromide and bromine. Bromate reactions with natural and synthetic gastric juices have been well documented in literature [6]. In addition, potassium bromate is a strong oxidizing agent with redox potential of 1.44 volts in acid medium [7]. Probably because of this reason bromate [Br(V)] is widely used as an oxidizing agent in synthetic as well as in analytical chemistry. Its oxidizing ability can be compared with reagents such as Ce (IV) [8], potassium iodate [9], sodium periodate [10-12], N-bromoacetamide [13-28] and N-bromosuccinimide [29-31], *etc.* have been earlier used in oxidation of various compounds.

In past several decades, potassium bromate has been widely used for the oxidation of a wide range of compounds [32-34]. Banerji and Negi [35] described the kinetics of oxidation of some aldoses and amino sugars by potassium bromate in hydrochloric acid medium. The reactions appear to proceed through the intermediate formation of bromate esters followed by the decomposition of the esters to give products. Hydrogen ion accelerated the rate of each reaction.

EXPERIMENTAL

Glycylglycine (E. Merck, analytical grade) was purified by column chromatography and used in experiment. Potassium bromate obtained from E. Merck with highest purity and analytical grade used as received, in stock solution. Acetic acid (E. Merck, analytical grade) was purified [36,37] by refluxing over chromium trioxide and acetic anhydride. The solid that separated out was filtered off and the filtrate distilled in an all glass quick fit apparatus and the fraction distilled at 118 °C was collected and used for all experiments. All other chemicals were of analytical grade.

Kinetics and measurements: The kinetic studies were carried out under pseudo-first order conditions with glycylglycine concentrations always greater than the concentration of $KBrO_3$. The progress of the reaction was monitored by estimating the unreacted concentration of $KBrO_3$ by iodometrically using freshly prepared starch as an indicator.

Stoichiometry: Stoichiometry studies were carried out under the conditions $[KBrO_3] >> [GG]$ in the presence of $Hg(OAc)_2$. The reaction was allowed to go to completion and the unreacted $KBrO_3$ was estimated iodometrically. It was found that one mole of glycylglycine required two moles of $KBrO_3$.

$$2HBrO_3 + H_2NCH_2\text{-}CONH\text{-}CH_2COOH \longrightarrow 2HCOOH + 2CO_2 + 2NH_4^+ + Br_2 + H_2O$$

Product analysis: The products of oxidation of glycylglycine were identified as HCOOH, NH_3 and CO_2. Formic acid was detected by conventional spot tests [38], while ammonia was identified by Nessler's reagent [39] and carbon dioxide was detected by gas evolution apparatus.

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AN EFFICIENT FUZZY LOGIC BASED EDGE DETECTION ALGORITHM

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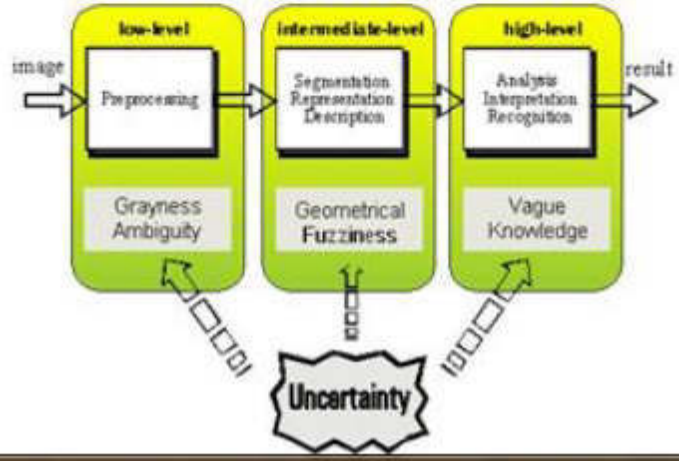
Abstract— **Fuzzy techniques allow a new perspective to model uncertainties due to the uncertainty of gray values present in the images .In previous Various Edge detection algorithm has been proposed in the literature for extracting the edges from the image. After emerging the fuzzy logic concept, a lot of Researcher of image processing shifted their attention towards the fuzzy logic concept and its applicability in the field of image processing. This paper presents an efficient fuzzy edge detection technique with parameters such as histogram; threshold and noise removing are carried out by using MATLAB R2015. This approach gives improved results than traditional edge detection techniques. Result of this technique is compared with various standard techniques like Sobel, Prewitt and Canny edge detection.**

Index terms- **Fuzzy Edge Detection, fuzzy rule, digital image processing, fuzzy classification, image segmentation, fuzziness.**

I. INTRODUCTION

The main purpose of edge detection in image processing is dimensional data from the real world in order to produce numerical or symbolic information [2]. In a color image, individual RGB value difference greater than threshold values. Edge detection may depend on the first derivative or the second derivative of the image intencitity values.



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Technical Note

Comparative study of old and new versions of treatment planning system using dose volume histogram indices of clinical plans

Gangarapu Sri Krishna[1,2], Vuppu Srinivas[1], K. M. Ayyangar[3], Palreddy Yadagiri Reddy[2]

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ABSTRACT

Recently, Eclipse treatment planning system (TPS) version 8.8 was upgraded to the latest version 13.6. It is customary that the vendor gives training on how to upgrade the existing software to the new version. However, the customer is provided less inner details about changes in the new software version. According to manufacturer, accuracy of point dose calculations and irregular treatment planning is better in the new version (13.6) compared to the old version (8.8). Furthermore, the new version uses voxel-based calculations while the earlier version used point dose calculations. Major difference in intensity-modulated radiation therapy (IMRT) plans was observed between the two versions after re-optimization and re-calculations. However, minor difference was observed for IMRT cases after performing only re-calculations. It is recommended TPS quality assurance to be performed after any major upgrade of software. This can be done by performing dose calculation comparisons in TPS. To assess the difference between the versions, 25 clinical cases from the old version were compared keeping all the patient data intact including the monitor units and comparing the differences in dose calculations using dose volume histogram (DVH) analysis. Along with DVH analysis, uniformity index, conformity index, homogeneity index, and dose spillage index were also compared for both versions. The results of comparative study are presented in this paper.

Key words: Conformity index; dose spillage index; dose volume histogram; homogeneity index; treatment planning version; uniformity index

Introduction

Aim

The aim of this study is to validate the new version (13.6) of Eclipse™ treatment planning for AAA algorithm after upgrading from old version (8.8).

From time to time, treatment planning system (TPS) users accept the vendor's latest version of treatment planning system. Most customers will not do any quality assurance (QA) to assess the performance of new version of TPS with respect to old version. Recently, Ojala *et al.*[1] quantified the dose difference between two versions of Acuros algorithms from AXB10 to AXB11 version (Varian Medical Systems, Palo Alto, CA). In their study, AXB11 was compared with AXB10 on the dose calculation accuracy. However, no general conclusion was made that the dose calculation accuracy of the AXB10 would be inferior to the AXB11, except in air cavities. The deviations between the two versions of the algorithm in the dose volume histogram (DVH) analysis were generally small. Performance of dose calculation in lung stereotactic body radiotherapy[2] was

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www.ijcto.org

Dosimetric analysis of 3D-conformal radiotherapy and intensity modulated radiotherapy for treatment of advanced stage cervical cancer: A comparative study

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Original Article

Abstract

Purpose: The purpose of this study is to analyze the dosimetric parameters of three dimensional conformal radiotherapy (3DCRT), intensity modulated radiotherapy (IMRT) with seven and nine fields (7F-IMRT, 9F-IMRT) in selected advanced stage cervical cancer cases. **Methods:** Fifteen cases of cervical cancer (IIB to IIIB) were selected for retrospective analysis. All the cases were previously treated with 3DCRT technique with prescribed dose of 50 Gy in 25 fractions. For this study, plans with seven fields IMRT and nine fields IMRT were generated for all patients following Radiation Therapy Oncology Group (RTOG) guidelines. The plans were compared on the basis of planning target volume (PTV) coverage (dose to 1%, 5%, 95% and 99% of target), maximum dose and mean dose to organs at risk (OARs) and also doses at different volumes of OARs. Apart from this, uniformity index (UI), homogeneity index (HI), conformity index (CI) and dose spillage index (R50%) were also calculated with respect to PTV coverage. **Results:** The average dose value of PTV coverage for all three techniques were comparable and all the DVH indices for 7field IMRT (UI (1.04±0.01), HI (0.07 ±0.02), CI (0.75±0.03) and R50% (4.47±0.36)) were better than 3DCRT and 9F-IMRT techniques. All OAR doses were significantly reduced in 7F- IMRT compared to 3DCRT and 9F- IMRT. The target volumes ranged from 769.2 ml to 1375.6 ml with average target volume of 1071.9 ml (SD: 205.38 ml). **Conclusion:** This study showed that significant dose reduction to OARs could be achieved with seven field IMRT plans by maintaining the PTV coverage compared to 3DCRT or 9F- IMRT for treating cervical cancer in advanced stages particularly from IIB to IIIB.

Keywords: Three dimensional conformal radiotherapy, Intensity modulated radiotherapy, Organs at risk, Uniformity index, Conformity index, Homogeneity index, Dose spillage index.

1. Introduction

The most common cancer in women is carcinoma of cervix.[1] In Worldwide, carcinoma of cervix is the fourth most common for females and the seventh most common cancer overall.[2] The Radiation treatment for cervical cancer includes combination of teletherapy and brachytherapy. There are much more advancements in the radiation treatment planning. In early 1990s, three dimensional conformal radiotherapy using CT images was the standard method to deliver radiation. Subsequently, more advanced technology IMRT was innovated in the late 1990s. In IMRT, the intensity of each beam is modified with the help of multileaf collimators (MLC) using inverse planning algorithms to treat the entire tumor while sparing critical structures. IMRT is the basis for all the new techniques like IGRT, VMAT and other modern techniques(SRS and SRT). A number of studies showed the benefit of IMRT over conventional external beam therapy.[3-5] Apart from

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PMID: 28144113

Clinical implications of Eclipse analytical anisotropic algorithm and Acuros XB algorithm for the treatment of lung cancer

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Abstract

The aim of the present study was to investigate the dose-volume variations of planning target volume (PTV) and organs at risks (OARs) in 15 left lung cancer patients comparing analytical anisotropic algorithm (AAA) versus Acuros XB algorithm. Originally, all plans were created using AAA with a template of dose constraints and optimization parameters, and the patients were treated using intensity modulated radiotherapy. In addition, another set of plans was created by performing only dose calculations using Acuros algorithm without doing any reoptimization. Thereby, in both set of plans, the entire plan parameters, namely, beam angle, beam weight, number of beams, prescribed dose, normalization point, region of interest constraints, number of monitor units, and plan optimization were kept constant. The evaluated plan parameters were PTV coverage at dose at 95% volume (TV95) of PTV (D95), the dose at 5% of PTV (D5), maximum dose (D_{max}), the mean dose (D_{mean}), the percent volume receiving 5 Gy (V5), 20 Gy (V20), 30 Gy (V30) of normal lung at risk (left lung- gross target volume [GTV], the dose at 33% volume (D33), at 67% volume (D67), and the D_{mean} (Gy) of the heart, the D_{max} of the spinal cord. Furthermore, homogeneity index (HI) and conformity index were evaluated to check the quality of the plans. Significant statistical differences between the two algorithms, $P < 0.05$, were found in D95, D_{max}, TV95, and HI of PTV. Furthermore, significant statistical differences were found in the dose parameters for the OARs, namely, V5, V20, and V30 of left lung-GTV, right lung (D_{mean}), D33, and D_{mean} of the heart, and D_{max} of the spine, respectively. Although statistical differences do exist, the magnitude of the differences is too small to cause any clinically observable effect.

Key words: Acuros algorithm, analytical anisotropic algorithm, conformity index, homogeneity index, intensity modulated radiotherapy, planning target volume coverage

Introduction

The algorithm used for dose calculation plays a very important role in delivery of dose to patients undergoing radiation treatment.[1] The beam configuration of analytical anisotropic algorithm (AAA) involves precalculated Monte Carlo data to determine all parameters to match the measured beam data.[2] The AAA calculation uses accurate Monte Carlo-based three-dimensional pencil beam convolution

Magnetic, ferroelectric, and spin phonon coupling studies of $Sr_3Co_2Fe_{24}O_{41}$ multiferroic Z-type hexaferrite

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K. Rama Reddy,[1] V. G. Sathe,[2] and V. Raghavendra Reddy[2]
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The magnetic, Raman, ferroelectric, and in-field ^{57}Fe Mössbauer studies of polycrystalline multiferroic $Sr_3Co_2Fe_{24}O_{41}$ are reported in this paper. From the magnetization studies, it is observed that the sample is soft magnetic in nature with low temperature magnetic spin transitions like longitudinal to transverse conical structure around 130 K and change in magnetic crystalline anisotropy from conical to planar structure at 250 K. Ferroelectric studies of the sample exhibit the spontaneous polarization at low temperature. Strong spin phonon and spin lattice coupling is observed through low temperature Raman spectroscopy. From the in-field ^{57}Fe Mössbauer spectroscopy, spin up and spin down site occupations of Fe ions are calculated in the unit cell. *Published by AIP Publishing.*
[http://dx.doi.org/10.1063/1.4960444]

I. INTRODUCTION

Magnetoelectric (ME) multiferroic materials exhibit magnetic and ferroelectric orders simultaneously. In these materials, magnetism is controlled by electric field and the electric polarization by magnetic field. This phenomenon is studied widely, both experimentally and theoretically due to their potential applications in information technology like spintronics and multibit memory storage device technology.[1–5] $BiFeO_3$ has become a famous multiferroic at room temperature, but the magnetoelectric coupling becomes too weak.[6] The magnetoelectric multiferroic material $TbMnO_3$, in which the polarization is produced by the magnetic order, has become an interesting magnetoelectric multiferroic material from theoretical and application point of views.[7] There are plenty of materials showing the multiferroic property at low temperatures, and they are not useful for practical applications.[8,9]

In recent years, the hexaferrites with long wavelength magnetic structure have become very interesting due to their potential applications in this field. Hexaferrites are classified into six types, namely, M, W, Y, Z, X, and U, depending on their chemical formula and magnetic structure. The unit cell of these hexaferrites consists of S [$Me^{2+}Fe_4O_8$, where Me is divalent metal ion], T [$(Me)_2Fe_8O_{14}$], and R [$MeFe_6O_{11}$] blocks having tetrahedral and octahedral environments in the unit cell.[10] In these hexaferrites, Y-Type $Ba_{0.5}Sr_{1.5}Zn_2Fe_{12}O_{22}$ shows the magnetoelectric property at low temperatures in which the polarization is induced by the external magnetic field. This can be explained through the spin current or Dzyaloshinskii–Moriya (DM) interaction where the polarization is induced by the interaction between the non-collinear spins through spin–orbit coupling.[11] However, some other Y-type hexaferrites like $Ba_2Mg_2Fe_{12}O_{22}$ and $BaSrZnCoFe_{11}AlO_{22}$ are showing spontaneous polarization at low temperatures.[12,13]

The Z-type hexaferrites belong to the P 6_3/mmc space group with lattice parameters a = b = 5.8 and c = 52 Å, and the magnetic structure consisting of four S blocks, two R blocks, and two T blocks can be described as RSTSR*S*T*S*, where * indicates that the corresponding block rotates 180° along the c-axis. The unit cell consists of 10 inequivalent crystallographic sites, $12k_{VI}$, $2d_V$, $4f_{VI}$, $4f_{IV}$, $4e_{VI}$, $4e_{IV}$, $2a_{VI}$, $4e_{VI}$, $4f^*_{IV}$, and 12^*k_{VI}, in which the Fe and metal ions are occupied.[14] The Z-type hexaferrite $Sr_3Co_2Fe_{24}O_{41}$ (SCFO) sintered in oxygen atmosphere is reported as room temperature multiferroic with field induced polarization, and the same sample sintered in air atmosphere displays the low temperature field induced polarization.[15] In contrast to these results, Wu *et al.*[16] reported that the same sample sintered in oxygen atmosphere shows room temperature multiferroic property with spontaneous polarization. The SCFO belongs to the ferroxaplana family in which the magnetic moments lies in the c-plane of unit cell at room temperature with soft magnetic nature. The Co_2 Z-type hexaferrites have three major changes in magnetic crystalline anisotropy (MCA) from cone to plane at 220 K and plane to uniaxial at 480 K, respectively.[10] The magnetic structure of the hexaferrites plays an important role in its multiferroic behaviour.

The spin phonon coupling is also an important aspect in the magnetoelectric multiferroic materials to understand the magnetoelectric phenomena. In hexaferrites, there are only a few studies on the spin phonon coupling till date. In this paper, we have reported the polycrystalline $Sr_3Co_2Fe_{24}O_{41}$ multiferroic hexaferrite sintered in air atmosphere and studied the magnetic behaviour along with Mössbauer studies and spin phonon coupling through temperature dependent Raman spectroscopy. To confirm the spontaneous polarization from the dipoles, we have studied temperature dependent P-E and PUND (positive up and negative down) with different delay times.

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Radiological health assessment due to gamma radiation levels of natural radioactivity of soil in vicinity of Nichahoma lignite belt, Kashmir Valley

Mudasir Ashraf, C. Anu Radha [1], Shakeel Ahmad [3], Sajad Masood [3], Rayees Ahmad Dar [4], V. Ramasubramanian [1], and P. Yadagiri Reddy [5]

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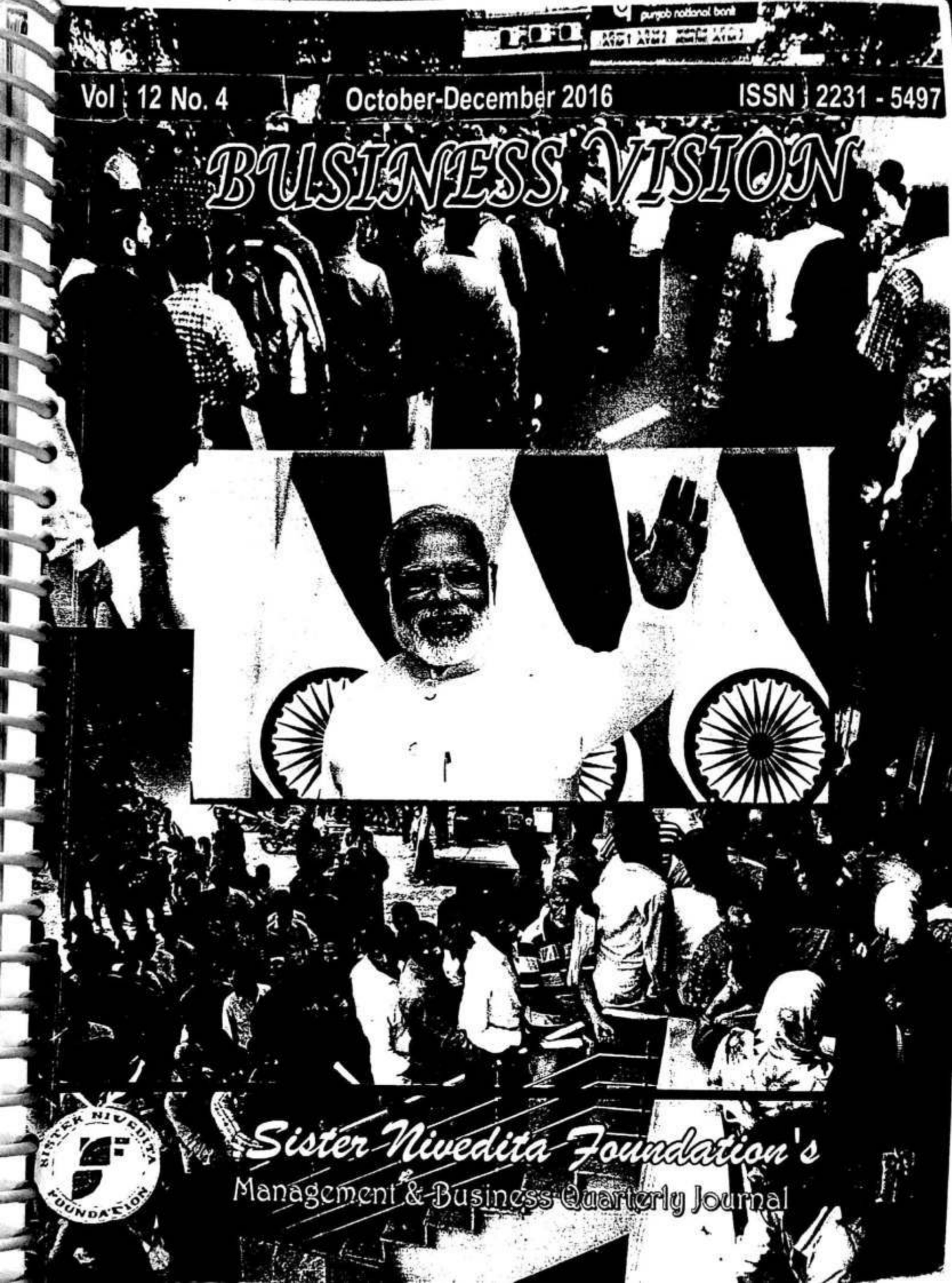

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Management & Business Quarterly Journal

SEBI's Regulations – the enforcement dimension

Securities Exchange Board of India (SEBI was set up in 1988 and has since then been instrumental in regulating the securities market with great efficiency, integrity and transparency. Today, India can boast of two national stock exchanges that have a market capitalization of greater than 1 trillion UD$, and are among the top ten globally. As per the latest GDP figures market – market capitalization to GDP ratio stands is 83 way above the 10 year average of 76[1]. This ratio also known as Buffet indicator forewarns of an impending bubble in the Indian stock-market, assuming that the GDP figures are correctly capturing the economy[2]. In such a scenario the role of the securities market regulator becomes even more critical. It is against this back-drop that an attempt has been made in this paper to study SEBI's enforcement regulations and activities. Also as SEBI had been assessed under the Financial Sector Assessment Program (FSAP) of IMF and World Bank in 2013, this study covers only the developments that have taken place after it.

***Dr. Vinita Sharma,** Assoc. Prof., Dept. of Business Management, PG Centre, AV College of Arts, Science & Commerce, Hyd.*

Introduction:

The very nature of securities transactions and markets, require strong regulations to protect the investors; ensure that the markets are fair, efficient and transparent; and to reduce systemic risk to the extent possible. International Organization of Securities Commissions (IOSCO) is an international body recognized as the global standard setter for the securities sector. Its members are the main financial regulator from each country. It has 414 members[3] from over 100 different countries that together regulate more than 95 percent of the world's securities markets. It has developed a comprehensive set of objectives and principles of Securities Regulation (IOSCO Principles) for members to adopt. It also helps member countries assess their level of compliance with these principles under its Financial Sector Assessment Program (FSAP) undertaken jointly by IMF and World Bank.

The Securities and Exchange Board of India (SEBI) is the principal regulator for securities markets in India. It regulates 8,594 registered brokers; 35,246 sub-brokers, 8,717 FPI's, 858 Depository Participants, 18 Designated Depositories Participants, 1,301 Clearing Members, 189 Merchant Bankers,

[1] Jun 9, 2016, Economic Times article "Take guard it smells like a bubble buffett indicator rings alarm bells for d street" available at http://economictimes.indiatimes.com/markets/stocks/news/take-guard-it-smells-like-a-bubble-buffett-indicator-rings-alarm-bells-for-d-street/articleshow/52666432.cms

[2] Jan 29,2016, F.Business "Why Raghuram Rajan doesn't trust India's GDP numbers" article available at http://www.firstpost.com/business/why-raghuram-rajan-doesnt-trust-indias-gdp-numbers-2603304..html.

[3] As on Dec 10, 2016, IOSCO has 207 members: 125 ordinary members, 18 associate members, and 64 affiliate members – data available at https://www.iosco.org/

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Bromination of Anisoles Using N-Bromophthalimide: A Synthetic and Kinetic Approach

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ABSTRACT: N-Bromophthalimide (NBP)-triggered bromination of aromatic compounds has been studied in the presence of aqueous acetic acid. Reaction Kinetics indicated first order in [NBP] and zero order in [Anisole]. The reactions afforded very good yields of corresponding bromo derivatives under kinetic conditions. The mechanism of the reaction is explained through the formation of acetyl hypobromite due to the interaction of NBP and acetic acid, which in turn reacts with anisole to afford a bromo derivative of anisole. © 2015 Wiley Periodicals, Inc. Int J Chem Kinet 1–8, 2015

INTRODUCTION

Bromination of aromatic compounds is an industrially important and fundamental chemical transformation in synthetic organic chemistry. Bromoaromatic compounds are used as precursors for the synthesis of a wide number of organometallic compounds, agrochemicals, and pharmaceuticals, and some of the aromatic bromides are known to exhibit significant antibacterial properties [1–5]. Several insecticides, herbicides, pesticides, and medicinally and pharmaceutically active molecules carry bromo functionality [6]. Molecular bromine is generally used in nuclear bromination, which generates toxic and corrosive HBr as a side product. Unused (excess) molecular bromine and the liberated HBr cause hazardous and harmful environment when sent to the drain [7–9]. However, the need for bromo aromatic compounds has led the chemists to develop alternative environmentally safe and ecofriendly bromination protocols [10]. Nath and Chaudhry reported ecofriendly and environmentally benign protocol for bromination of aromatic compounds, using KBr/H_2O_2 in the presence of boric acid as a recyclable catalyst [11]. Potassium bromide in the presence of poly(4-vinylpyridine)-supported bromate in nonaqueous solution is used as a mild reagent for efficient bromination of aromatic compounds [12]. Monobromination of electron-rich aromatic compounds at room temperature has been achieved using $CuBr_2$ [13,14]. Regioselective bromination of aromatic compounds has been found using KBr in the presence of benzyltriphenylphosphonium peroxodisulfate in acetonitrile medium under reflux condition [15]. Oxybromination of activated aromatics has been afforded using shape selective zeolite such as HZSM-5, CrZSM-5(30) [16] as a catalyst, H_2O_2 as an oxidant, and KBr as a bromine source in AcOH

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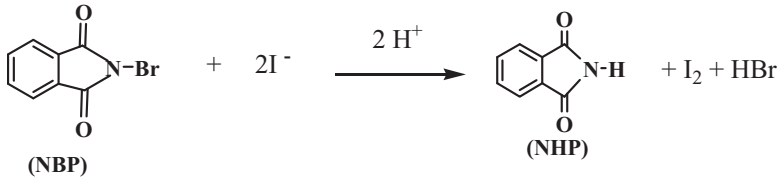
medium. In recent past, the Vilsmeier–Haack reagent [17] has been reported for efficient bromination of aromatic compounds using KBr under a conventional and solvent-free mortar–pestle condition from our laboratories. Even though few protocols have also been developed for bromination of aromatic compounds using *N*-bromosuccinimide (NBS) [18–23], such studies are not found using *N*-bromophthalimide (NBP) as a brominating agent. In this part of the work, we would like to present certain synthetic and kinetic aspects of bromination of anisoles using NBP. Nevertheless, we have recently reported kinetics of oxidation of few organic compounds [24].

EXPERIMENTAL

The reagents employed in this study were (Merck, India) and NBP (Sigma Aldrich, India). All the chemicals used were of analytical grade. Acetic acid was refluxed with chromic oxide and acetic anhydride for 6 h and then fractionally distilled according to literature procedures [25]. All aqueous solutions were prepared in doubly distilled water. Freshly prepared NBP solution was used throughout the experiment. Stock solution of NBP was prepared by dissolving a requisite amount of NBP in acetic acid. The NBP content estimated iodometrically using standard solution of sodium thiosulfate ($Na_2S_2O_3$) and 1% solution of freshly prepared starch as an indicator. The concentration of NBP was calculated using the following stoichiometric equation:



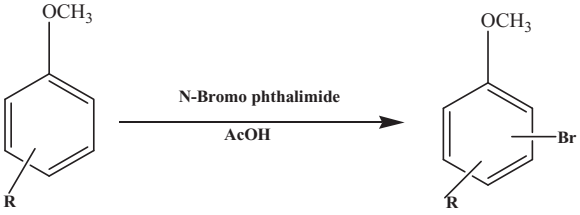
$$I_2 + 2\,Na_2S_2O_3 \rightarrow 2\,NaI + Na_2S_4O_6$$

Table I Bromination of Aromatic Compounds by NBP under Conventional Conditions

Entry	Substrate	Product	Yield (%)
1	Anisole	4-Bromoanisole	85
2	4-Chloroanisole	2-Bromo-4-chloro anisole	78
3	4-Nitroanisole	2-Bromo-4-nitro anisole	74
4	4-Methylanisole	2-Bromo-4-methyl anisole	79
5	4-Ethylanisole	2-Bromo-4-ethyl anisole	76
6	4-Methoxyanisole	2-Bromo-4-methoxy anisole	75
7	4-Bromoanisole	2,4-Dibromo anisole	71
8	4-Isopropyl anisole	2-Bromo-4-isopropyl anisole	73

Reaction time: Conventional 10–13 h.

evaporated under vacuum, purified with column chromatography to get a pure product (Table I).



General Procedure for Conventional Synthesis of Bromo Aromatic Compounds Using NBP

A centimolar (0.01 mol) organic substrate, 0.01 mol of NBP and about 0.002 mol $Hg(OAc)_2$ and solvent (AcOH) were taken in a previously cleaned round bottom flask and stirred for about 9–13 h at room temperature. After completion of the reaction, as confirmed by TLC, the reaction mixture was treated with $NaHCO_3$ solution, followed by the addition of ethyl acetate. The organic layer was separated, dried over Na_2SO_4, and

Stoichiometry and Product Analysis

The stoichiometry of the reaction was determined by taking known excess of [NBP] over [anisole] in aqueous acetic acid media at desired temperature. The progress of the reaction was followed for several days to ensure the completion of the reaction. The unreacted [NBP] in aliquots was estimated every day till a constancy in the titer value is obtained. Final analysis indicated that the reactants ratio [NBP]: [anisole] was found to be 1:1. The products of the

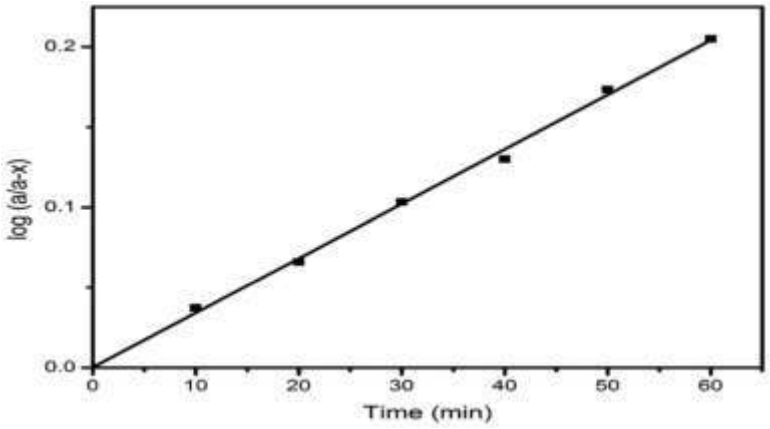


Figure 1 Order in [NBP] in the oxidation of anisole by NBP.

reactions were characterized by mass and H-NMR techniques and compared with literature reports. The NMR spectra were recorded on a Bruker Avance DEX 500 and 300 MHz instrument. The spectra were measured in $CDCl_3$ relative to TMS (0.00 ppm). As typical examples, data for **2-b**romo-4-methylanisole and 2-bromo-1-methoxy-4-nitrobenzene are given below.

2-Bromo-4-methylanisole : 'H-NMR 6 2.27 (3H, s), 3.86 (3H, s), 6.79 (lH, d, $J = 8.2$ Hz), 7.06 (lH, dd, $J = 2.2$ and 8.2 Hz), 7.36 (lH, d, $J = 2.2$ Hz).

2-Bromo-1-methoxy-4-nitrobenzene **:** mp 108–110°C; 1H NMR ($CDCl_3$, 400 MHz) δ 8.75 (d, $J =$ 4 Hz, 1H), 8.45 (dd, $J_1 = 8$ Hz, $J_2 = 4$ Hz, 1H), 7.23 (d, $J = 8$ Hz, 1H), 4.10 (s, 3H).

Kinetic Method

The reaction mixture contained requisite amounts of thermally equilibrated NBP, anisole, and mercuric acetate solutions prepared in aqueous acetic acid. Kinetics of the bromination reactions were studied under pseudo–first-order conditions with [anisole] >>> [NBP] in a constant temperature bath at a desired temperature. The reaction was initiated by adding NBP as the last component to rest of the reactant solutions, viz. anisole, Hg(II) acetate, salt, etc. The progress of the reaction was followed by iodometric determination of the unreacted [NBP] in aliquots of the reaction mixture withdrawn into aqueous KI solutions at regular time intervals. The iodine liberated was titrated against the standard sodium thiosulfate solution using a starch indicator. Mercuric acetate was used in the reaction mixture as a bromide scavenger, which did not affect the rate of reaction to any significant extent, which was observed by earlier workers in NBS- and NBP-initiated reactions [26,27]. Under the conditions [anisole] >>> [NBP], the linear plot log $(a/(a-x))$ versus time, passing through the origin indicated the order in [NBP] to be unity (Fig. 1).

Variation of [anisole] over a wide concentration range under pseudoconditions did not alter the rate constant to any significant extent. This observation can be seen from the small magnitude of slope (<0. 2) presented in the logarithmic plot of rate constant (k') as a function of [anisole] (Fig. 2). This observation may suggest a "zero"-order kinetics (actual order $n = 0.11$) in [anisole].

According to the theory of absolute reaction rates (Eyring's theory), the rate constant k and free energy of activation $\Delta G^{\#}$ correlated as

$$k = (RT/Nh)\exp(-\Delta G^{\#}/RT)$$

where R is the gas constant, h is the Plank's constant, N is the Avogadro's number, and T is the temperature in an absolute scale. The above equation is used to calculate the free energy of activation ($\Delta G^{\#}$) at various temperatures [28]. Accordingly, free energy of activation $\Delta G^{\#}$ has been calculated from the rearranged form of Eyring's equation at different temperatures:

$$\Delta G^{\#} = RT\ \ln(RT/Nhk)$$

Free energy of activation ($\Delta G^{\#}$) values thus obtained were further used in the Gibbs–Helmholtz plot of ($\Delta G^{\#}$) versus T, using the following equation for the evaluation of enthalpy of activation ($\Delta H^{\#}$) and entropy of activation ($\Delta S^{\#}$), as shown in Table III.

$$\Delta G^{\#} = \Delta H^{\#} - T\Delta S^{\#}$$

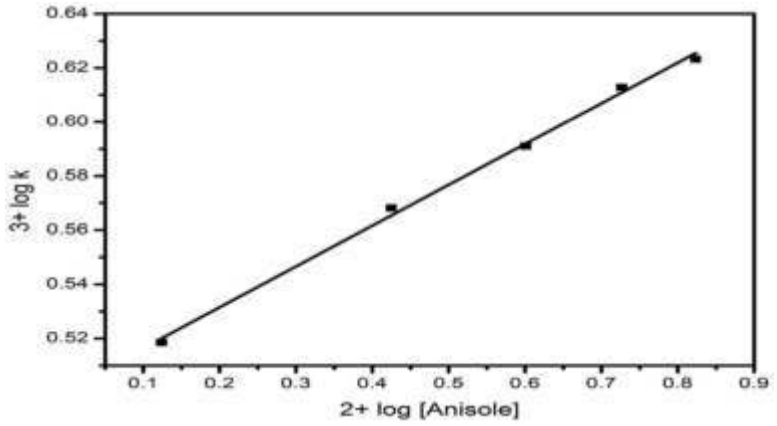


Figure 2 Effect of [anisole] on k' in the NBP–anisole reaction.

RESULTS AND DISCUSSION

NBP possesses a highly polar N–Br bond in the lines of other its structural analogue NBS. Therefore, NBP has also been reported as a good oxidizing and brominating agent by several earlier workers [24,26], and [27]. Because of large polarity of >N–Br bond NBP, like other similar *N*-halo imides such as NBS, may exist in various forms in acetic acid medium, i.e., free NBP, protonated NBP ($NBPH^+$), HOBr, $(H_2OBr)^+$, Br^+, and CH_3COOBr according to the following equilibria:

$$NBP + H_2O \rightleftharpoons HOBr + NHP \quad (1)$$

$$NBP + H^+ \rightleftharpoons NHP + Br^+ \quad (2)$$

$$NBP + H^+ \rightleftharpoons (NBHP)^+ \quad (3)$$

$$HOBr + H^+ \rightleftharpoons (H_2OBr)^+ \quad (4)$$

Reactive Species and Mechanism of Reaction

***First Approach (Case-1) Considering "Zero"-Order Kinetics in* [Anisole].** Effects of various additives such as $[HClO_4]$ and $[NaClO_4]$ may throw light on the influence of [Brønsted acid], ionic strength (μ), and dielectric constant (D) on the reaction rate are generally useful to analyze and ascertain the active species and thereby propose a plausible mechanism. A kinetic study in different compositions of binary solvent mixtures of acetic acid and water provided information of about the variation of dielectric constant (D) on the reaction rate.

Table II Effect of Variation of Different Additives on the Rate of NBP Bromination of Anisole

	Additive			
10^2 [NHP] (mol dm^{-3})	10^2 [$NaClO_4$] (mol dm^{-3})	HOAc% (v/v)	[$HClO_4$] (mol dm^{-3})	10^3 k'
0.6	–	50	–	2.8
1.3	–	50	–	2.7
2.0	–	50	–	2.8
2.6	–	50	–	2.9
3.3	–	50	–	3.1
–	0.6	50	–	2.9
–	1.3	50	–	2.7
–	2.0	50	–	2.8
–	2.6	50	–	2.6
–	3.3	50	–	2.5
–	–	54	–	2.9
–	–	40	–	3.2
–	–	27	–	3.4
–	–	14	–	3.5
–	–	7	–	3.9
–	–	50	0.005	2.8
–	–	50	0.020	2.9
–	–	50	0.026	3.0
–	–	50	0.033	3.1
–	–	50	0.330	3.0
–	–	50	1.50	3.1

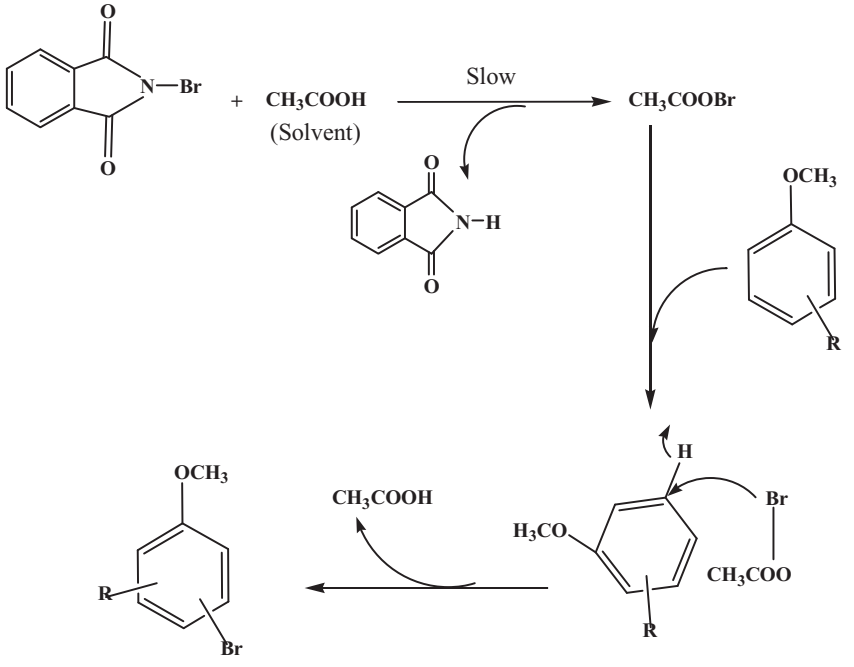
10^3[NBP] = 1.00 mol dm^{-3}; 10^2 [anisole] = 1.00 mol dm^{-3}; 10^3 [$Hg(OAc)_2$] = 2.00 mol dm^{-3}; temperature = 308 K.

Rate data presented in Table II show that none of the above additives had any significant effect on the reaction rate. However, a marginal decrease in the rate due to an increase in the HOAc% (v/v) could be attributed

Table III Kinetic and Activation Parameters for the Bromination of Anisoles by NBP

Substrate	Temperature (K)	k (min)	$\Delta G^{\neq}$ (kJ/mol)	Gibbs-Helmholtz $\Delta G^{\neq} = \Delta H^{\neq} - T\Delta S^{\neq}$ Equation with R^2	$\Delta H^{\neq}$ (kJ/mol)	$-\Delta S^{\neq}$ (J/K/mol)
Anisole	308	0.013	86.56	$y = 143.39x + 42475$, $R^2 = 0.9944$	42.47	143.39
	313	0.016	87.41			
	318	0.021	88.18			
	323	0.030	88.70			
	328	0.038	89.50			
p-Cl anisole	308	0.014	86.43	$y = 134.55x + 45106$, $R^2 = 0.9864$	45.10	134.55
	313	0.017	87.30			
	318	0.022	88.04			
	323	0.033	88.43			
	328	0.041	89.24			
p-NO_2 anisole	308	0.014	86.27	$y = 136.03x + 44373$, $R^2 = 0.9998$	44.37	136.03
	313	0.020	86.95			
	318	0.026	87.62			
	323	0.035	88.28			
	328	0.045	89.01			
p-CH_3 anisole	308	0.017	85.80	$y = 150.12x + 39679$, $R^2 = 0.9932$	39.67	150.12
	313	0.021	86.81			
	318	0.028	87.45			
	323	0.038	88.10			
	328	0.047	88.91			
p-C_2H_5 anisole	308	0.020	85.46	$y = 153.24x + 38259$, $R^2 = 0.9975$	38.25	153.24
	313	0.027	86.14			
	318	0.033	87.05			
	323	0.042	87.79			
	328	0.055	88.47			

10^3[NBP] = 1.00 mol dm^{-3}; 10^2 [anisole] = 1.00 mol dm^{-3}; AcOH = 50% (v/v); 10^3 [$Hg(OAc)_2$] = 2.00 mol dm^{-3}.



Where R= EWD or ED groups

Scheme 1 Mechanism of NBP-induced bromination.

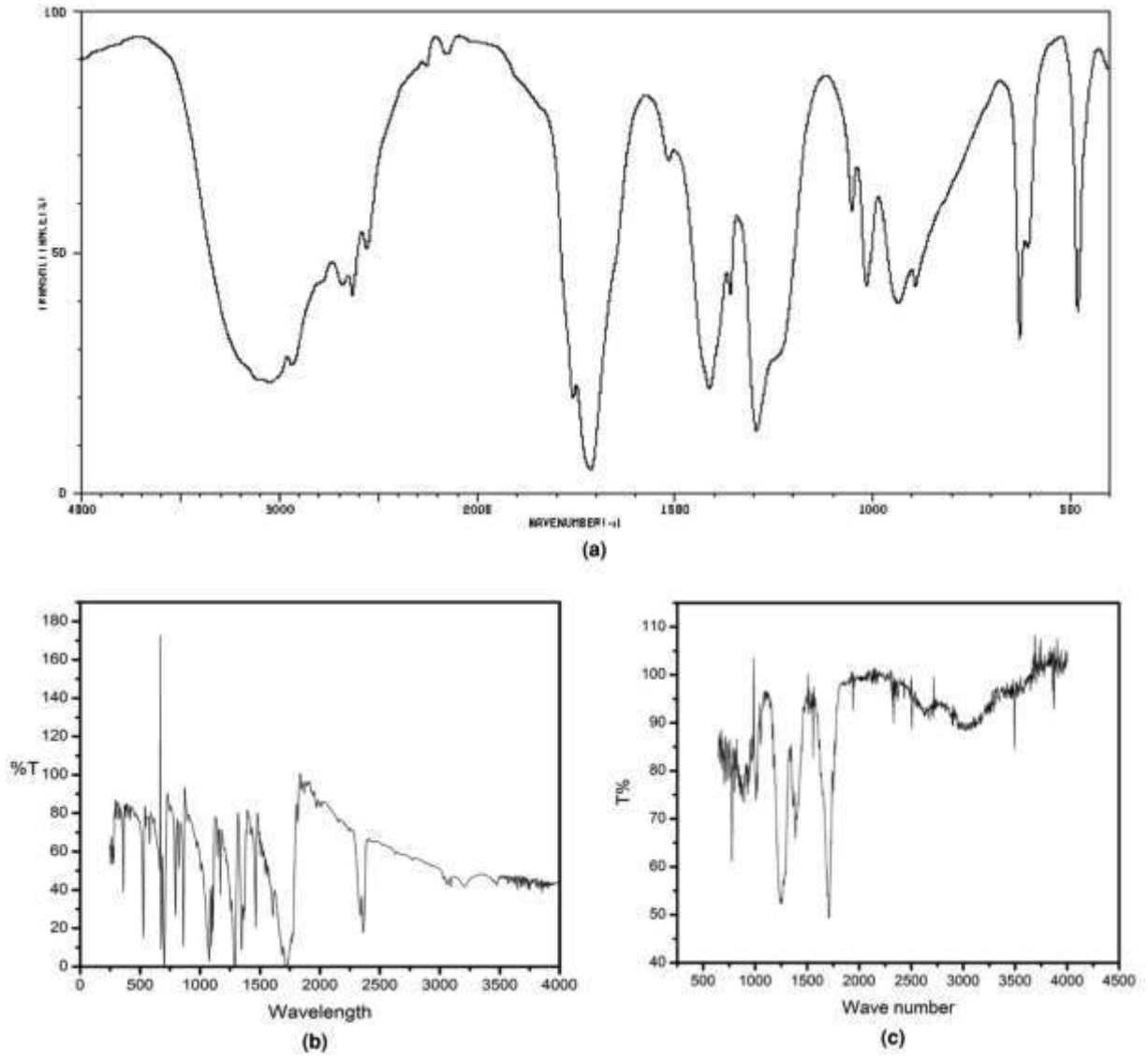
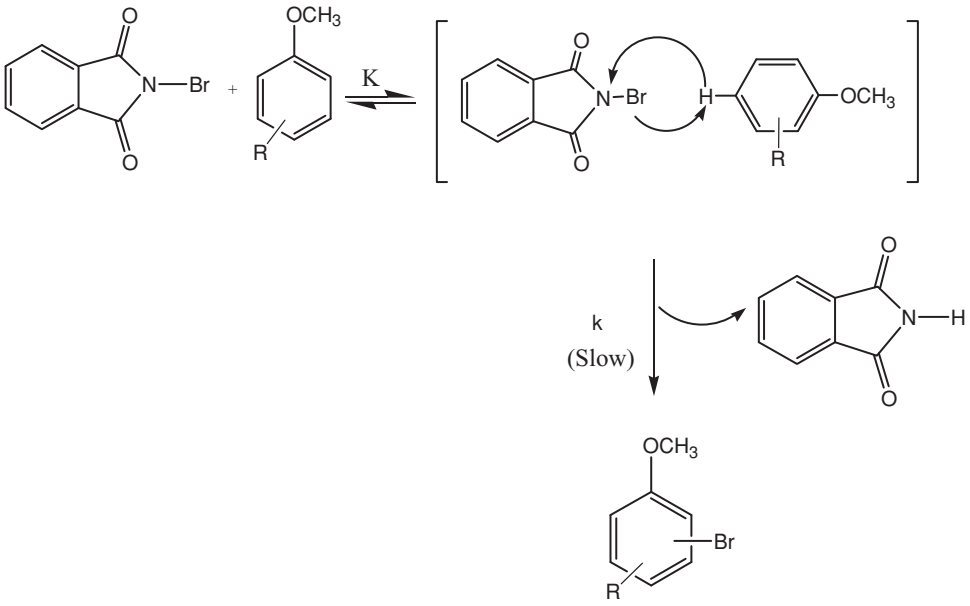


Figure 3 (A) IR spectrum of acetic acid(AcOH); (B) IR spectrum of NBP; (C) IR spectrum of (NBP+AcOH).

to the dimerization of acetic acid due to solvent–solvent interactions. If HOBr is assumed as the reactive species, the derived rate law should explain the negative effect of [phthalimide] according to equilibrium (i). But in the present study, the rate did not change with addition of phthalimide to the reaction mixture over a wide concentration range. Accordingly, participation of HOBr could be ruled out in the rate-limiting step. If protonated NBP $(NBPH)^+$ or $(H_2OBr)^+$ is taken as reactive species, the rate law should depict first-order kinetics with respect to $[H^+]$. Contrary to this aspect, our observation indicated that an increase in $[H^+]$ did not alter the rate to any significant extent, ruling out protonated NBP $(NBPH)^+$ or $(H_2OBr)^+$ is taken as a reactive species. On the other hand, observed negligible rate effects with the variation ionic strength, [NHP] and dielectric constant (Table II) may at best suggest the participation of NBP molecular species in the slow step. Since the order with respect to [anisole] is "zero," NBP might generate acetyl hypobromite (CH_3COOBr) due to solvent (CH_3COOH)–solute (NBP) interactions as shown in Eq. (5).

$$CH_3COOH + NBP \rightarrow CH_3COOBr + NHP \quad (5)$$

Acetyl hypobromite may further react with an aromatic compound through the in situ generated bromonium ion (Br^+) to afford a corresponding bromo derivative followed by the regeneration acetic acid as shown in Scheme 1. For the above mechanism, given in



Scheme 2 NBP-induced bromination of anisoles.

Scheme 1, the rate law comes out as

$$\text{Rate} = -\text{d[NBP]}/\text{d}t = k[\text{NBP}][\text{CH}_3\text{COOH}]$$

However, it is important to note that acetic acid is used as a solvent and its concentration is far greater than [NBP] and [anisole]. Therefore, the rate law simply comes out as

$$\text{Rate} = -\text{d[NBP]}/\text{d}t = k'[\text{NBP}]$$

The rate law is in consonance with the observed results such as first-order dependence on [NBP] and zero-order dependence on [anisole] (because, $n = 0.101$, very low $<<$ 1.0). Formation of acetyl hyprobromite is supported by IR and UV spectroscopic studies. The characteristic IR peaks of the carboxylic –OH group observed as as a broad band a in the range of 3000–2500 cm^{-1}(shown in Fig. 3A) underwent a substantial decrease in the intensity in the presence of NBP (Fig. 3C). Similarly, a sharp peak observed in the range of 2300–2400 cm^{-1} corresponding to the C–N moiety of NBP spectrum (Fig. 3B) also underwent a remarkable decrease in the intensity. These observations further strengthen our contention for the in situ formation of acetyl hyprobromite. Formation of acetyl hypobromite and its properties were also explored by Reilley et al [29] and Hatanaka and co-workers [30].

***Alternative Mechanism (Case-2) Considering Complex (Fractional) Order in* [Anisole].** Alternatively, for a spur of moment if we have a closer look into the observed kinetic data, it depicts very small differences in the reaction rates of the structurally different anisoles and also with an increase in the concentration of anisole. The order in [anisole] obtained as a small fraction ($n = 0.101$, very low $<<$ 1.0). By considering even this small fractional (complex) order in [anisole], the Michaelis–Menten type mechanism is proposed as shown in Scheme 2.

The rate law for the above mechanism can be written as

$$\text{Rate} = \frac{kK[\text{Anisole}][\text{NBP}]}{1 + K[\text{Anisole}]}$$

Reciprocal plots of $(1/k')$ versus 1/[anisole] afforded almost nearer decomposition constant (k) values (very small variations) in structurally different anisoles as substrates with the order of reactivity of anisoles was found to be in the following order: 4-ethylanisole > 4-methyl anisole > anisole > 4-chloroanisole > 4-nitroanisole. Hammett's plot of log k versus σ depicted very poor correlation ($R^2 = 0.69$) and small reaction constant ($\rho = -0.182$)**.** In view of these reasons, the "Michaelis–Menten-type mechanism discussed under Case-2" may not be more likely than the given in Scheme 1. Hence the authors feel that the reaction follows zero-order kinetics in [anisole] and follows Scheme 1 as the most plausible mechanism.

CONCLUSIONS

The NBP reaction with anisoles in aqueous acetic acid afforded very good yields of corresponding bromo derivatives in 10–13 h. The reaction followed first-order kinetics in [NBP] and zero order in [anisole], indicating the decomposition of NBP in the rate-limiting step to generate acetyl hypobromite, which in turn affords a bromo derivative of anisole. The bromination of anisoles is governed by the transfer of bromine (as Br(I)) to acetic acid.

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COMPETENCY MAPPING AMONG COLLEGE TEACHERS : PROBLEMS AND PROSPECTS

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IMPACT OF THE FACULTY COMPETENCES ON THE ACADEMIC PERFORMANCE OF THE POSTGRADUATE STUDENTS: A CASE STUDY ON THE STUDENTS OF GDC, SIDDIPET, MEDAK (D), TELANGANA, INDIA

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ABSTRACT

The teacher is a poten-tial divine being who is a respon-si-ble and account-able author-ity to trans-form the per-son-al-ity of the stu-dent in a use-ful, pur-po-sive and ascend-ing direc-tion. Qual-ity of teach-er gen-er-ates qual-i-fied stu-dents. The current case study investigates that the influence of the teacher's competencies on the academic performance of the students among higher education. A sample of 156 (60%) students was selected and used for the study using simple random sampling procedure. A structured questionnaire was used to gather data from various post graduate students of Government Degree and P.G.College ,Siddipet, Medak(D),Telangana, India, and the researcher analyzed the feedback of the students in statistical manner. Results indicate that Teachers' competencies like Qualification, subject knowledge, teaching experience, teaching skills, in-service trainings, research experience and academic co-operation with students had show greater influence on student achievement.

KEY WORDS

Teacher, Competencies, Student and Academic performance.

Introduction

Teachers are regarded as the most imperative knowledge-based factor that influences student's achievement levels. According to Adunola (2011) and Ganyaupfu (2013), teaching is a collaborative process which encompasses interaction by both learners and the lecturer. According to Akiri & Ugborugbo (2009), lecturer competence in teaching process is a multidimensional concept that measures numerous interrelated aspects of sharing knowledge with learners which include communication skills, subject matter expertise, lecturer attendance, teaching skills and lecturer attitude. Therefore, the competence of a lecturer is directly measured by students' academic achievements.

Review Literature

The famous and ancient book "**Arthashastra**",which is considered as the first book of competency mapping, written by **Arya chanakya**. It contains human aptitude, competency mapping models, intelligence quotient and emotional quotient and related to human behavior on work, logic and emotions.

According to **UNIDO** (2002) A Competency is a set of skills, related knowledge and attributes that allow an individual to successfully perform a task or an activity within a specific function or a job.

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Research Article

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Kinetics and mechanism of oxidation of ketoacids by N-bromophthalimide in aqueous acetic acid medium

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ABSTRACT

The kinetics and mechanism of oxidation of keto acids viz., Pyruvic acid (PA) and Levulinic acid (LA) by N-Bromophthalimide (NBP) in the presence of mercuric acetate have been investigated in aqueous acetic acid medium at 35°C. The reaction follows first order kinetics each in [NBP] and [keto acid]. The activation parameters have been evaluated. Based on the observed kinetic results, a probable mechanism has been proposed.

Keywords: Kinetics, oxidation, keto acid, N-Bromophthalimide.

INTRODUCTION

The keto acids are especially important in biology as they are involved in the Krebs citric acid cycle and in Glycolysis. Keto acids are readily decarboxylated by several metallic and non-metallic oxidizing agents such as ceric sulphate, potassium permanganate, lead tetra acetate and hydrogen peroxide [1]. Pyruvic acid (PA) is one of the smallest biomolecule with a keto acid function. Previous studies of pyruvic acid oxidation by higher valent metal oxidants are rather limited in the literature [2-9]. In recent years, studies of the oxidation of various organic compounds by N-halo compounds in acidic medium have attracted considerable attention. They are the sources of a positive halogen and the mechanism of these reactions depends on the nature of the active oxidizing species, which may differ depending on the nature of halogen atom, the groups attached to the nitrogen atom and the reaction conditions [10-17]. However, no study involving pyruvic acid (PA) and levulinic acid (LA) with N-Bromophthalimide has been reported so far. Keeping these points in mind, we thought it appropriate to study the kinetics and mechanism of oxidation of keto acids, viz. pyruvic acid (PA) and levulinic acid (LA) in aqueous acetic acid medium with N-Bromophthalimide (NBP) in the temperature range of 308-328K.

EXPERIMENTAL SECTION

The reagents employed were Pyruvic acid and levulinic acid (Merck) and N-Bromophthalimide (Sigma Aldrich). All the chemicals used were of analytical grade. Acetic acid was refluxed with chromic oxide and acetic anhydride for 6 h and then fractionally distilled according to literature procedures [18].The solution of NBP was always prepared freshly and was standardized iodometrically. All aqueous solutions were prepared in doubly distilled water.

KINETIC METHOD

All kinetic measurements were performed under pseudo-first-order conditions with [keto acid] at least 10-fold in excess over [NBP] at a constant ionic strength (μ) were thermally equilibrated for an hour at the desired temperature. The reaction was initiated by the addition of previously thermostated solutions of NBP and keto acid solution of the

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Comparative Analysis of Some Algal Ferritins Belonging To Chlorophyta and Rhodophyta

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Abstract
Ferritin is the most important protein involved in the Iron metabolism and storage. Iron is an extremely important element whose function is involved in the oxygen transport and it participates in the electron transfer reactions and various redox potential reactions. Ferritin, the globular cytoplasmic protein is highly conserved and is involved in the regulation of the flow of iron into and out of the cell. The structural integrity of the protein makes it convenient to store 45,000 molecules of iron in it. In the current paper we have worked on the analysis of ferritin from different species of Algae using bioinformatics tools. Algal ferritins studies are undertaken with reference to some of the members of Chlorophyta and Rhodophyta. Chlamydomonas reinhardtii is a model member of Chlorophyta involving two unlinked genes FER1 and FER2 encoding ferritin sub-units. Comparative studies are performed in different classes of algae i.e. Chlorophyta and Rhodophyta to understand variations in ferritin sequences.

Key words- *Ferritin, electron transfer, Chlorophyta, Rhodophyta, FER1 and FER2.*

Introduction

Metal interactions with organic compounds are numerous in all living organisms. They are essential for many biochemical processes occurring within cells, and concern not only metabolism, but also some regulatory mechanisms of gene expression. Among metals, iron is of special interest because it is required in most of the cellular redox reactions and it is one of the major metals involved in electron transfer chains. However, its strong reactivity with oxygen makes it a difficult element to handle by aerobic organisms. Indeed, both its insolubility in the form of ferric hydroxides, or its toxicity through the Fenton reaction producing hydroxyl radicals (which are among the most chemically reactive species), have introduced evolutionary constraints in order to enable this metal to be safely utilized by living organisms [1]. The narrow efficient iron concentration required for cellular needs is strictly controlled by biological processes acting both at the transport and the storage levels. In multicellular organisms, transport mechanisms regulate iron traffic from uptake to long distance tissular distribution, and ultimately to subcellular allocation [2]. Although the structure of ferritins is highly conserved between plants and animals, their cellular localization differs. Furthermore, regulation of ferritin gene expression in response to iron excess occurs at the transcriptional level in plants, in contrast to animals which regulate ferritin expression at the translational level.
Iron is toxic in uncontained situations because it catalyzes the production of free radical. Thus iron in the cell is stored in **"FERRITIN"** [10].

In algae, ferritins are plastid-located proteins able to form a holosphere, which can contain up to 4500 Fe atoms. This process allows us to buffer free iron, making it available under a safe form, and reveals a key role for ferritin in iron homeostasis and protection against iron-mediated oxidative stress [4]. Pre-ferritin, with a plastid targeting sequence, is encoded by a multigene family in plants. Increased ferritin production in high-iron-supplied cells is accomplished, at least in part, by transcriptional regulation of one or more ferritin genes [5]. This pattern of expression is consistent with a role for ferritin as an iron storage molecule under conditions of iron overload[6]. Despite extensive studies conducted during the last decade, many factors regulating the expression of ferritin genes in plants remain unknown (Marek Figlerowicz *et.al.,* 2009).

Ferritins are a broad superfamily of iron storage proteins, found in all the living kingdom, except in yeast (Andrews et al., 2003; Briat et al., 2006; Arosio et al., 2008).
Three subclasses of these proteins can be defined:
(1) haem-free ferritins present both in pro- and eukaryotes;
(2) haem-containing bacterioferritins, found only in bacteria; and
(3) DNA binding proteins from starved cells (Dps), called miniferritins,

Present in prokaryotes (Smith, 2004). Ferritins and bacterioferritins are composed of 24 subunits whereas only 12 identical subunits form the Dps proteins. These subunits assemble in a spherical protein shell defining a central cavity able to

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SCREENING AND PURIFICATION OF ANTIBACTERIAL PROTEINS AND PEPTIDES FROM SOME OF THE MEDICINAL PLANTS SEEDS

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ABSTRACT

Antibiotics have been effective in treating infectious diseases, but resistance to these drugs has led to the emergence of new and the reemergence of old infectious diseases. For centuries, Indian spices have made a significant contribution both in the health care system and the food industry. Ancient Asian literature is a treasure of information related to the problems of health care and other environmental aspects. Bacterial strains used for the study was *S. aureus* (ATCC 25923), *E. coli* (ATCC 25922), *P. aeruginosa* (ATCC 27853) and *P. vulgaris* (ATCC 6380) were purchased from Hi-Media laboratories. Our results showed that various buffer pH have different protein extractability percentages after dialysis for the seed extracts used. The protein was extracted by sodium phosphate citrate buffer pH (7.2) highest concentration of the protein was found to (660µg/ml) in *Ammi majus* and the *lowest* was 160 µg/ml in . The highest protein concentration extracted by CTAB buffer pH (6.0) was found to be (640µg/ml) in *Ammi majus* and the lowest was 140 µg/ml in *Chichorium intybus.*

KEYWORDS: ***Medicinal plants, Antimicrobial Activity, Bacterial strains.***

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REASONS FOR CHOOSING CONTRACT MANUFACTURING ORGANIZATION IN PHARMACEUTICAL INDUSTRY

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ABSTRACT

During our survey from 2009 to 2012 we had found some different issues regarding outsourcing in Pharmaceutical companies which were beneficial and non-beneficial for large multi-national pharmaceutical companies as well as smaller ones, other side of our study we had found there were some advantages of Contract Manufacturing Organization in Pharmaceutical Industry. The study included of about 40 pharmaceutical outsourcing companies. Survey was conducted from 2009 to 2012.

KEYWORDS: Contract Manufacturing Organization (CMO), Outsourcing, Pharmaceutical Industries, Food and Drug Administration (FDA).

INTRODUCTION

"A company which assigns some of its non-core activities to third party is known as outsourcing". Outsourcing is an important activity preformed in the pharmaceutical companies which provide essential information regarding how essentially things are done rather than what is to be done. The process by which an organization contracts with another individual or company to get some of its work done is known as outsourcing. Normally it is non-core aspects of the business that are outsourced. Outsourcing will save time, which is often critical because any delay in production processes, batch releases, or obtaining approvals from regulatory bodies can severely damage a company's prospects. The opposite of outsourcing is called insourcing which entails bringing processes handled by third-party firms in-house, and is sometimes accomplished via vertical integration. However, a business

can provide a contract service to another business without necessarily insourcing that business process.

By way of outsourcing some of the client's faces some hurdles with third party service providers such as communication barrier, threat to intellectual property rights, quality problem, etc. Though cost is one issue which is important factor; however there are two other critical factors such as intellectual property and quality & safety issues. Of these the most important one is intellectual property rights. Some of the third party service providers selling their clients patents rights to other companies and manufacture & sell drugs that rightfully belong to someone else.

The Food and Drug Administration issued approvals for 12,000 plants in India and China. The employment in American pharmaceutical industry came down 5 percent from the last year and India's pharmaceutical industry grew 13 percent in case of hiring employees. According to EconomyinCrisis.com, 1,742 drugs were recalled in 2009 and just 338 drugs were recalled in 1999 due to outsourcing. Even the simple over-the-counter drugs have been recalled because of safety concerns, including Proctor & Gamble Decongestant Nasal Spray and Johnson & Johnson's Children's Tylenol, Tylenol Arthritis Pain Caplets, Extra Strength Tylenol Rapid Relief Gels. The latter was traced to a fungicide that originated from a Puerto Rican plant.

While some of those products were manufactured in the U.S however their components came from outside the U.S., and due to the lack of manpower at the FDA, much of it goes unchecked until a problem is discovered. "Up to 40 percent of the drugs Americans take are imported, and up to 80 percent of the active pharmaceutical ingredients in those drugs come from foreign sources," Food and Drug Administration Commissioner Margaret Hamburg, M. D., said, according to *The Buffalo News.*[1]

A Contract Manufacturing Organization (CMO) is otherwise known as Contract Development and Manufacturing Organization (CDMO). CRO is meant for research & development and CMO is meant for manufacturing.

Services offered by CMOs are follows,

Pre-formulation, formulation development, stability studies, method development, pre-clinical and Phase I clinical trial materials, late-stage clinical trial materials, formal stability, scale-up, registration batches and commercial production.

EVOLUTION OF CMO

In the pharmaceutical industry, if R & D has to outsource that can be provided through contract research organizations (CROs) and for outsourcing manufacturing than contract manufacturing organizations (CMOs). Now a day contract development and manufacturing organizations (CMOs) is coming if any pharmaceutical company is looking for a comprehensive single-source provider from drug development through commercial manufacture.[2]

ADVANATGES OF CONTRACT MANUFACTURING ORGANIZATION

1) Cost Saving

Taking into consideration the huge costs involved in plant and equipment, the pharmaceutical companies can save a lot of money by outsourcing some part of their activities to third party vendors. Outsourcing to CMO's can reduce the overall costs by 30% to 35%.

2) Focus on core competencies

Outsourcing to a CMO allows the pharmaceutical client to expand its technical resources without increased overhead. The client can then manage its internal resources and costs by focusing on core competencies and high-value projects while reducing or not adding infrastructure or technical staff. Virtual and specialty pharmaceutical companies are particularly well-suited to CDMO partnerships, and big pharmaceutical companies are beginning to view relationships with CDMOs as strategic rather than tactical.

3) Less Capital Investment

Working with a CMO also limits a client's upfront capital investment for drug development, thus minimizing a project's cost. By concentrating resources with a single-source provider, the outsourcing client can minimize technical transfer of projects or products, thereby reducing unforeseen costs and potentially speeding new products to market.

4) Geographic Advantage

If the CMO is located in another country and if it is in close vicinity with the API supplier, it will provide tremendous logistical savings.

5) Flexibility

Based on the current business trends, work scheduling can be reshuffled easily without affecting work on other products.[3]

REVIEW OF LITERATURE

Our study were also correlated with the other studies carried out by,

Dustin Ensinger's objective in his article "Pharmaceutical Outsourcing threats" was the U.S. pharmaceutical industry is no longer immune to the outsourcing phenomenon, which poses major risks for American consumers. The author specifies India is becoming a major destination for American pharmaceutical companies seeking to boost their bottom line. Taking their cues from other American multinational corporations, they are doing so by outsourcing their manufacturing to the Indian subcontinent according to *The New York Times*. The author also pointed a comment in his article raised by Panos Kalaritis, the chief operating officer of Irix Pharmaceuticals, a Florence, S.C., contract research and manufacturing company, that "Cost is one issue, and yes it is important, but there are two other critical factors: intellectual property and quality and safety issues," in *The New York Times*. He has mentioned that Americans were losing jobs and Indians were gaining jobs due to outsourcing. The employment in American pharmaceutical industry came down five percent from the last year and India's pharmaceutical industry grew 13 percent in case of hiring employees. The Food and Drug Administration issued approvals for 12,000 plants in India and China. He has mentioned the quality issue where last year, 1,742 drugs were recalled and just 338 drugs were recalled in 1999. Even the simple over-the-counter drugs have been recalled because of safety concerns. Even some of those products were manufactured in the U.S however their components came from outside the U.S., and due to the lack of manpower at the FDA, much of it goes unchecked until a problem is discovered.

"Up to 40 percent of the drugs Americans take are imported, and up to 80 percent of the active pharmaceutical ingredients in those drugs come from foreign sources," Food and Drug Administration Commissioner Margaret Hamburg, M. D., said, according to *The Buffalo News*.[1]

Daya Mukherjee was insisted in his article that "Look Before You Sign Your Outsourcing Contract" He explained the factors that a firm needs to look for before signing the outsourcing contract. He explained clearly that the contract should typically cover scope of work, little flexibility in the contract, problem resolution such as monetary compensation,

problem escalation, terminating the contract procedures, repatriation clause etc., terms & conditions agreed upon, the service level agreement, and non-disclosure agreement should signed by both the parties.[4]

Mak Jawadekar was sharing his experiences in his article "Outsourcing Steps in India-The biggest advances in the Indian CMO arena" which was published in contractpharma.com. The author was sharing his experiences at some partnership meeting with many Indian companies during the Bio Asia 2009 Conference in Hyderabad with Pfizer's senior management - including two Presidents of Pfizer Global R&D (Dr. John LaMattina and Dr. Martin Mackay. He also had had a meeting with the President of India, Mrs. Pratibha Patil. She was very interested in knowing how global pharma companies like Pfizer could help patients in India get access to the modern medicines.

A rising global acceptance of generics, coupled with increased outsourcing of manufacturing by "Big Pharma" to lower-cost locations, has benefited the export-focused Indian pharma companies. The author was predicting that contract manufacturing volumes outsourced to India, as well as certain partnerships and alliances by multinational companies (MNCs) with quality Indian majors will increase. He was giving example of Aurobindo Pharma and Claris Lifesciences have entered into alliances with large pharma for specific products, including upfront license fees.

He was pin pointing that India-focused pharma companies will continue to benefit from steady domestic growth, with a consequent overall boost in volumes and capacity utilization. Pricing pressures - due to a greater-than-expected increase in competition - could offset some of the anticipated improvements in profitability. He showed the difference between existing players as well as new entrants into the generics space. This will lead to key risk factor for future margins. Even regulatory issues could also have an impact, primarily with regard to approvals for new products and any tightening in quality controls. The author was saying that India is well-placed in strong manufacturing base - both in formulations, as well as in key areas (bulk drugs and APIs). India has the highest number of FDA-approved plants outside of the U.S. Many global financial firms have predicted that rising purchasing power and increasing penetration of health insurance reform will support strong growth in India's domestic formulations business in the long term.

Makarand (Mak) Jawadekar most recently served as Director, Portfolio Management and Performance at Pfizer Global R&D, until February 2010, when he opted for an early retirement after 28 years at Pfizer Inc. He currently serves on several companies' advisory boards and also consults with bio/pharmaceutical companies for global outreach in emerging market regions.[5]

"Global Pharmaceutical Contract Manufacturing Market to Reach US$40.7 Billion by 2015" published in PharmaManufacturing.com, 2011. The author in this article conveyed that the global market for pharmaceutical contract manufacturing witnessed robust growth in recent years, and the future continues to hold tremendous prospects for the industry. Several developed countries in the globe began scouting for ways to minimize expenditure on drugs. Most of the pharmaceutical companies were trying to minimize cost of drugs which directly lead to evaluate opportunities for manufacturing outsourcing.

Even at the time of recession the pharmaceutical contract manufacturing industry, overall market maintained a positive growth posting only a moderate slowdown in growth. However, a drop in venture capital funding due to the recession has compelled many pharmaceutical and biotechnology companies to cut down on spending, affecting the fortunes of contract manufacturers worldwide. This resulting to several projects were kept on hold and new project starts were delayed, cascading the impact of the pharmaceutical industry to the outsourcing industry as well.

The author emphasizing manufacturing capacity constraints are only one of the reasons for outsourcing. Pharmaceutical manufacturing entails sophisticated technology (cGMP synthesis and scale up, impurity profiling, lyophilization) and strict regulatory compliance (good manufacturing practices - GMP). Outsourcing such activities to Contract Manufacturing Organizations (CMOs) enables a pharma company to expedite its R&D, and thus realize the potential revenues. Moreover, CMOs are increasingly offering a wide range of value-added services, which make PCMO an indispensable opportunity to pharma companies.

The author listed major players profiled in the report include Althea Technologies, Catalent Pharma Solutions, Dishman Pharmaceuticals and Chemicals Ltd, HAUPT Pharma AG, Jubilant Life Sciences Limited, Kemwell Pvt. Ltd, NextPharma, Nipro Corp., Patheon Inc., Royal DSM N.V., among others.[6]

Ed Silverstein in his article "Pharmaceutical Contract Manufacturing Vendors See Increases in Revenue", healthtechzone.com, 2013 published in h.ealthtechzone.com was referring the quotation led down by Frost & Sullivan "The market for pharmaceutical contract manufacturing earned $13.43 billion in revenue during 2012 and it may go as high as $18.49 billion in 2017" The article also noted that how pharmaceutical companies concentrate on "core competencies," which has led to more outsourcing and helped the pharmaceutical contract manufacturing market. The sector includes: injectable doses, liquid doses, semi-solid doses and solid doses.

The author conveyed the statement led down by Frost & Sullivan analyst Aiswariya Chidambaram "Investments and capacity expansions in the injectable dose formulation segment are in the near future, as it is likely the most significant source of income for the global pharmaceutical contract manufacturing industry," and "Cytotoxics manufacturing, in particular, offers immense growth potential, given the demand from the cancer research and therapy segments."

In this article the author noted that the analysis done by Frost & Sullivan that how the pharmaceutical contract manufacturing market is "highly fragmented with many contract manufacturing organizations (CMOs) relying on one client for more than 50 percent of their revenue."

"Coupled with huge tax incentives and lower inventories for low-volume products, this creates immense pricing pressures for CMOs," the firm said in a statement.

The United States and Europe are major markets for outsourcing finished dose formulations and sterile preparations, Frost & Sullivan said.

The author has given example of a U.S.-based company is Pharma Tech Industries (PTI), a contract manufacturer and packager. It is believed to be largest contract processor and packager of powder products. It makes over one billion effervescent tablets a year, "moves over 50 million pounds of powders yearly, and the numbers for their cotton swab and injection molding production lines are equally large," according to a report from Advantage Business Media.

In addition, Asian CMOs are often used for active pharmaceutical ingredients, intermediates and generics. Also, because of lower costs, Asian CMOs, such as in China, India and

Singapore, could become “favorable destinations, particularly for solid dose formulations,” Frost & Sullivan said.

Watch out for more acquisitions and alliances in the sector, too.

"Consolidation in the form of acquisitions and strategic alliances to gain access to new, emerging markets and niche segments will be crucial for both small and large CMOs," Chidambaram predicts. "Large CMOs can broaden their geographic presence, while small CMOs can leverage the technical expertise and resources of large CMOs to enlarge their footprint.".[7]

Aiswariya Chidambaram/Frost in their article **“**Contract manufacturing to reach $18 bn by 2017” published in Biospectrum.com, 2013 was specifying that “Global pharmaceutical contract manufacturing market earned revenue of $13.43 billion in 2012 and is estimated to reach $18.49 billion in 2017”, expanding market for solid dose, liquid and semi-solid dose and injectable dose formulations, according to a report by Frost and Sullivan.

According to the analysis firm, cost benefits and pharmaceutical companies' desire to focus on their core competencies has created an increasing need for outsourcing and spurred the global pharmaceutical contract manufacturing market.

The analysis firm also specifying that expiring blockbuster drug patents will reduce manufacturing capacity utilization rates and leads to outsourcing further.

The source of income for the global pharmaceutical contract manufacturing industry would be expansion and investments in the injectable dose formulation segment are in the near future the analysis firm healthcare research analyst, Ms Aiswariya Chidambaram confirms. Cancer drugs manufacturing gives growth potential and demand from cancer research and therapy segment. The global pharmaceutical contract manufacturing market remains highly fragmented with many contract manufacturing organizations (CMOs) relying on one client for more than 50 percent of their revenue.

Coupled with huge tax incentives and lower inventories for low-volume products, this creates immense pricing pressures for CMOs,” The analysis firm insisted that Currently, the US and Europe are major markets for outsourcing finished dose formulations and sterile preparations, whereas Asian CMOs are preferred destinations for active pharmaceutical ingredients,

intermediates and generics. However, due to the immense cost benefits, Asian CMOs, like in India, China and Singapore, will likely emerge as favorable destinations, particularly for solid dose formulations.

"Large CMOs can broaden their geographic presence, while small CMOs can leverage the technical expertise and resources of large CMOs to enlarge their footprint." Ms Chidambaram concluded.[8]

OBJECTIVES

1. To identify the reasons for choosing CMO in Pharmaceutical Industry.
2. To examine the advantages of CMO in Pharmaceutical Industry.

HYPOTHESIS

Whether outsourcing to CMO's are beneficial to the pharmaceutical industries?

METHODOLOGY

Data Collection Method

The study depends on primary and secondary source.

Primary Source Data

Primary data has been collected through the direct personal investigation in the form of the questionnaire and Indirect oral investigation in the form of personal interview.

Secondary Source Data

Secondary Data will be driven from, books, journals, company records, company web sites.

RESEARCH DESIGN

Research design means the basis of defining the research problem. The preparation of the design of the research project is popularly known as the research design. The study aims to find out the reasons for choosing Contract Manufacturing Organization in Pharmaceutical Industry.

Sample Design

For the purpose of the study, a sample of 40 pharmaceutical outsourcing companies taken into consideration, 25 pharmaceutical outsourcing companies taken into consideration of which 10 pharmaceutical companies were into blend of both outsourcing and in sourcing

within the India and 15 pharmaceutical outsourcing companies taken from outside of the India mostly from USA.

RESULTS

40 Different companies were representing for advantages of CMO in pharmaceutical outsourcing. 100 % of companies were showing for Cost Saving & for Focus on Core Competencies, 75 % of companies were showing for Less Capital Investment & Geographic advantage and 70 % of the companies were showing for Flexibility**.**

Table 1. advantages of contract manufacturing organization.

Particulars	Number of Companies	Percentage
Cost Saving	40	100
Focus on Core Competencies	40	100
Less Capital Investment	30	75
Geographic advantage	30	75
Flexibility	28	70
No of Companies To Be Studied	**40**	**100**

Figure 1. advantages of contract manufacturing organization.

DISCUSSIONS AND CONCLUSION

Based on our study we would like to conclude that outsourcing to CMO's in pharmaceutical industries plays a significant role not only in Cost Saving, Focus on Core Competencies, Less Capital Investment and Geographic advantage but also in Flexibility. It provides a big support to pharmaceutical and biotechnology industries for completion of their projects hassle free.

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CHALLENGES IN CONTRACT MANUFACTURING ORGANIZATIONS IN PHARMACEUTICAL INDUSTRY

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ABSTRACT

During our survey from 2009 to 2012 we had found some different issues regarding outsourcing in Pharmaceutical companies which were beneficial and non-beneficial for large multi-national pharmaceutical companies as well as smaller ones, other side of our study we had found there were some Challenges in Contract Manufacturing Organization in Pharmaceutical Industry. The study included of about 40 pharmaceutical outsourcing companies.

KEYWORDS: Contract Manufacturing Organization, Outsourcing, Pharmaceutical Industries, Food and Drug Administration, Good Manufacturing Practice.

INTRODUCTION

A Contract Manufacturing Organization (CMO) is otherwise known as Contract Development and Manufacturing Organization (CDMO). CRO is meant for research & development and CMO is meant for manufacturing.

Services offered by CMOs are follows, Pre-formulation, formulation development, stability studies, method development, pre-clinical and Phase I clinical trial materials, late-stage clinical trial materials, formal stability, scale-up, registration batches and commercial production.

EVOLUTION OF CMO

In the pharmaceutical industry, if R & D has to outsource that can be provided through contract research organizations (CROs) and for outsourcing manufacturing than contract

manufacturing organizations (CMOs). Now a day contract development and manufacturing organizations (CMOs) is coming if any pharmaceutical company is looking for a comprehensive single-source provider from drug development through commercial manufacture.[1]

Contract manufacturing means a firm manufactures the products for another hiring company or firm as it is a form of outsourcing. In this type of business the hiring firm approaches the contract manufacturer with a new design or formula to develop and create a new project with the help of contract manufacturer. The contract manufacturer will decide the quotation based on land, labor, capital, and organization, generally they investigate in market and make a research on the quotation of material and tools. Production of goods by one firm, under the label or brand of another firm. Contract manufacturers provide such service to several (even competing) firms based on their own or the customers' designs, formulas, and/or specifications. Also called "Private Label Manufacturing."[2]

Contract manufacturing organizations (CMOs) offer a wide array of manufacturing services to the pharmaceutical and biotechnology industries. These services can range from production of small quantities of materials for R&D purposes, larger amounts for clinical study usage and ultimately full-scale production for commercial purposes. The global contract manufacturing market primarily includes solid and liquid dosage forms and injectables. The growing use of generic drugs and complex pharmaceutical products has also induced many CMOs to offer active pharmaceutical ingredient (API) manufacturing services to their clients. In 2011, total global spending on contract manufacturing reached $31.9 billion according to a 2012 Informal report entitled "The CMO Market Outlook to 2017". The CMO industry had experienced double digit growth in the past two decades and that trend is expected to continue for the next five years. By 2017, the size of the global contract manufacturing market is expected to grow to about $63 billion. While, in recent years, there has been a steady growing demand for API manufacturing, solid dosage formulation remains the largest segment of the CMO industry by revenue. The solid dosage market is expected to expand over the next five years at an annual rate of 12.5% and as much as $55 billion will be spent by 2017 on CMO-based solid dosage manufacturing.[3]

Challenges In Contract Manufacturing Organization

Many pharmaceutical companies, big and small, have been outsourcing work to contract research organizations (CRO's) and contract manufacturing organizations (CMO's). There

are several advantages and disadvantages. In spite of these numerous advantages, there are many challenges to working with CRO's and CMO': The bottom line of every project is "getting work done" and "meeting with the timeline".

1. Quality control

In the early years of the relationship, it is difficult to understand the company value system of the CRO and CMO, which will generate conflicts (despite making a quality agreement). Once a quality issue is raised, an investigation and resolution can become time-consuming, expensive and a headache.

2. Accountability

If things are not in place and fall through the cracks, it is easy to criticize personnel within the CMO. However, this might have long-term ramifications because the project manager has to continue to work with the CMO staff to ensure operational streamlining.

3. Flexibility

One assumes unlimited flexibility with CRO's and CMO's. It is assumed that the production schedule with the CMO can be modified, shifted, decreased or increased whereas the reality of the experience could be the total opposite.

4. Paperwork

The CMO may be running a very lean operation and may not have staff to keep track of paperwork. This may pose difficulties when filing the product with the FDA.

5. Supply chain issues

Being a small company, the CMO may not have well developed procurement and systems. This could put the corporation at a major disadvantage.

6. Intellectual property risks

Even after signing an appropriate contract, one may face breaches in intellectual property safe-keepings. CMO's work with many clients and in spite of many precautions taken, the probability of critical product information being leaked is greatly increased. There is an increased probability of leaking of critical product information.

7. Acquisition and management change

After a long-term relationship and understanding, the CMO could be acquired by another company. All the previous relation-building may go down the drain. In some cases, the value system of the new management may not be on the same wavelength with the previous management. If the company has to change the CMO at this point, the company has to spend on product transfer (time and money expenditure).

If the CRO or CMO are in another country, there are several other barriers such as:

A. Language – They may not be fluent in American-English.

B. Time – A difference of 6 to 12 hours due to time-zone changes is very common

C. Cultural variation – A difference in work hours and holidays.

D. Corruption – People in the parent company may not have knowledge to deal with the corrupt officials in another country. The difference in the value system can generate major conflicts and face challenges to company policies.

E. Patent issues and local politics

F. Exploitation of a multinational company: It is hard to plan to minute details and the contract written could be more general. As the project develops, if the parent company does not have a physical presence in the foreign CMO, the CMO will tend to exploit and the company can lose the cost advantage.[4]

REVIEW OF LITERATURE

Our study were also correlated with the other studies carried out by, Nick Taylor in his article was conveying "US firm offering modular plant leases as alternative to CMOs" published in outsourcing-pharma. com, 2011. The author was conveying in his article that US firm offering modular plant leases as alternative to CMOs. He was mentioning that Biologics Modular is leasing its mobile production facilities to help clients make FDA regulated drugs without fixed plants. Biologics Modular thinks the model will appeal to research park innovator biopharm that need access to flexible and affordable GMP (good manufacturing practice) production capacity.

The author in his article he was mentioning the quotation given by Clark Byrum, Jr, president and CEO of Biologics Modular "*The current business model for drug manufacturing companies is changing, and as we see more offsite research and development, there is a growing need for affordable quality facilities*".

The author was conveying that Biologics Modular is pitching the model as an alternative to outsourcing to contract manufacturing organisations (CMOs). Instead of outsourcing manufacture of clinical trial materials biopharma can have a Biologics Modular facility temporarily installed at their site to handle production.

The facilities are manufactured by Biologics Modular at its site in Indiana before being qualified and validated. Clients also receive support with process validation, GMP quality control and regulatory strategies.

By taking this modular, pre-constructed, pre-tested approach to facility design Biologics Modular claims it can deliver a plant within 20 weeks. Validation and commissioning is said to take days.

The author was explaining about Building a facility, which are housed in steel shipping containers. Inside the containers Biologics Modular installs pre-constructed, pre-tested modules, like giant Lego pieces, to equip the production facility.

Once constructed the facility is relocated to, for example, a leased light industrial warehouse. When the plant is no longer needed it can be decommissioned and in most cases, Biologics Modular will handle the removal.[5]

Dustin Ensinger's objective in his article "Pharmaceutical Outsourcing threats" was the U.S. pharmaceutical industry is no longer immune to the outsourcing phenomenon, which poses major risks for American consumers. The author specifies India is becoming a major destination for American pharmaceutical companies seeking to boost their bottom line. Taking their cues from other American multinational corporations, they are doing so by outsourcing their manufacturing to the Indian subcontinent according to *The New York Times*. The author also pointed a comment in his article raised by Panos Kalaritis, the chief operating officer of Irix Pharmaceuticals, a Florence, S.C., contract research and manufacturing company, that "Cost is one issue, and yes it is important, but there are two other critical factors: intellectual property and quality and safety issues," in *The New York Times*. He has mentioned that Americans were losing jobs and Indians were gaining jobs due to outsourcing. The employment in American pharmaceutical industry came down five percent from the last year and India's pharmaceutical industry grew 13 percent in case of hiring employees. The Food and Drug Administration issued approvals for 12,000 plants in India and China. He has

mentioned the quality issue where last year, 1,742 drugs were recalled and just 338 drugs were recalled in 1999. Even the simple over-the-counter drugs have been recalled because of safety concerns. Even some of those products were manufactured in the U.S however their components came from outside the U.S., and due to the lack of manpower at the FDA, much of it goes unchecked until a problem is discovered.[6]

"Up to 40 percent of the drugs Americans take are imported and up to 80 percent of the active pharmaceutical ingredients in those drugs come from foreign sources," Food and Drug Administration Commissioner Margaret Hamburg, M. D., said, according to *The Buffalo News*.

Dore explained in his article "cut your outsourcing risks." He explained toll processing relationships, with respect to chemicals, active pharmaceutical ingredients and finished drug products. In this article he explained that both large and small pharma companies turned to toll processing after commercial drug product introduction, typically when manufacturing tasks had become routine. The Toll processing relationships resources dealing with the operational, safety, contractual, legal, regulatory and other aspects of these transactions is quite limited. He explained even the U.S. Food and Drug Administration's (FDA) 2001 Guidance for Industry Q7A Good Manufacturing Practice Guidance for Active Pharmaceutical Ingredients provides only that, all contract manufacturers should comply with the Good Manufacturing Practices (GMP) defined in this guidance, companies should evaluate any contractors. to ensure GMP compliance of the specific operations occurring at the contractor sites, a written and approved contract or formal agreement between a company and its contractors should be made available defining in detail the GMP responsibilities, including the quality measures of each party, a contract should permit a company to audit its contractor's facilities for compliance with GMP, where subcontracting is allowed, a contractor should not pass to, a third party any of the work entrusted to it under the contract without the company's prior evaluation and approval of the arrangements, manufacturing and laboratory records should be kept at the site where the activity occurs and be readily available, changes in the process, equipment, test methods, specifications or other contractual requirements should not be made unless the contract giver is informed and approves the changes. He finally concluded that cut your outsourcing risks.[7]

Daya Mukherjee was insisted in his article that "Look before You Sign Your Outsourcing Contract" He explained the factors that a firm needs to look for before signing the

outsourcing contract. He explained clearly that the contract should typically cover scope of work, little flexibility in the contract, problem resolution such as monetary compensation, problem escalation, terminating the contract procedures, repatriation clause etc., terms & conditions agreed upon, the service level agreement, and non-disclosure agreement should signed by both the parties.[8]

OBJECTIVES

1) To examine the challenges in CMO in Pharmaceutical Industry.
2) To examine the reasons for not choosing CMO in Pharmaceutical Industry.

HYPOTHESIS

Whether outsourcing is non-beneficial to the pharmaceutical industries?.

METHODOLOGY

Data Collection Method

The study depends on primary and secondary source.

Primary Source Data

Primary data has been collected through the direct personal investigation in the form of the questionnaire and Indirect oral investigation in the form of personal interview.

Secondary Source Data

Secondary Data will be driven from, books, journals, company records, company web sites.

RESEARCH DESIGN

Research design means the basis of defining the research problem. The preparation of the design of the research project is popularly known as the research design. The study aims to find out challenges in Contract Manufacturing Organization in Pharmaceutical Industry.

SAMPLE DESIGN

For the purpose of the study, a sample of 40 pharmaceutical outsourcing companies taken into consideration, 25 pharmaceutical outsourcing companies taken into consideration of which 10 pharmaceutical companies were into blend of both outsourcing and in sourcing within the India and 15 pharmaceutical outsourcing companies taken from outside of the India mostly from USA.

RESULTS

40 Different companies were representing for challenges in CMO in pharmaceutical outsourcing companies. 70% of companies were showing for Loss of Intellectual Property, 60% of companies were showing for Quality Control & Time Delays, 50% of the companies were showing for Flexibility and 25% of the companies were showing for Change in Management.

TABLE 1.

Particulars	Number of Companies	Percentage
Quality Control	24	60
Flexibility	20	50
Loss of Intellectual Property	28	70
Change in Management	10	25
Time Delays	24	60
No of Companies To Be Studied	**40**	**100**

Figure 1.

DISCUSSIONS AND CONCLUSION

We would like to conclude that though outsourcing in pharmaceutical industries plays an significant role in Cost Saving, focusing on drug discovery, Less Capital Investment, Geographic advantage and Flexibility however, there are other factors such as Quality Control, Flexibility, Loss of Intellectual Property, Change in Management and Time Delays were also very important which are to be considered by client before they outsources their non-core business activities. If an organization really wants to outsource their products/projects to CMO's then first they should make a survey about the third party service provider whether the employees are well qualified, they have capability to complete the job and whether they respect intellectual property rights. If the third party is unknown to the client then they should check the references about the third party. If all these issues are sort out then there won't be any of these lacunas in outsourcing and certainly CMO's can provide better solutions to their clients in many ways.

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Outline

Figures (6)

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Structural, electrical, magnetic and ^{57}Fe Mössbauer study of polycrystalline multiferroic $DyFeO_3$

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RESEARCH ARTICLE

PRELIMINARY INVESTIGATION OF NATURALLY OCCURRING RADIONUCLIDE IN SOME FIVE LOCALLY MANUFACTURED CEMENT TYPES COMMONLY USED IN KASHMIR VALLEY AS BUILDING MATERIAL

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ABSTRACT

The present study was aimed at the determination of specific activity of locally manufactured and commercially available five cement types used as building material in Kashmir valley, India by using a NaI (Tl) gamma ray spectrometer. The study envisages that the mean values of specific activity concentrations in the different analyzed cement samples were found to vary from 44.4±0.81 to 51.02±2.3 $Bqkg^{-1}$ for ^{226}Ra; 20.11±3.60 to 36.91±2.9 $Bqkg^{-1}$ for ^{232}Th and 25.29±1.42 to 55.78±2.81 $Bqkg^{-1}$ for ^{40}K, the mean value specific activity for ^{226}Ra in all the investigated cement brand were above the world average of 32 $Bqkg^{-1}$. The radiation hazard indices determined are well below the limits and all the analysed cement brands used in Kashmir valley meet the safety requirement and do not pose any radiological hazard to human health.

***Citation*:** Shakeel Ahmad, Mudasir Ashraf, Sajad Masood *et al*. 2015. "Preliminary investigation of naturally occurring radionuclide in some five locally manufactured cement types commonly used in Kashmir valley as building material", *International Journal of Current Research,* 7, (6), 16835-16839.

INTRODUCTION

One inescapable feature of life on the earth is exposure to the ionizing radiations. Ionizing radiation of the environment is the most ubiquitous form of exposure therefore determination of health risk of background radiation is of great importance in health physics (UNSCEAR, 2010). The main sources of the background radiation are cosmic and terrestrial radiations. Cosmic radiations include energetic particles produced by spallation reactions in the outer space of the atmosphere which penetrate into the earth's atmosphere and contribute as one of the main sources of background radiation. Interaction of these particles with atmosphere molecules may produce cosmogenic radionucleides. Long half lived radionuclides which were formed at the time of formation universe have formed terrestrial radionuclides which exist in air, soil, rocks, water and building materials. The terrestrial predominant radionuclides, with respect to absorbed dose in human, are ^{232}Th and ^{238}U are head of decay series in which radionucleides of the chain contribute to human exposure and increase total radiation on earth (UNSCEAR, 2000). Studies conducted on natural radioactivity have shown that the presence of potassium (^{40}K) and other daughter radionucleides from Thorium (^{232}Th) and Uranium (^{238}U) decay series in various components in the environment result in radiation exposure of the global population (El- Tahir, 2012). The primordial radionucleides are predominant in almost all raw and produced materials widely used in the building industries including; cement, brick, sand, tile, limestone, gypsum and those derived from rocks and soil (El- Tahir, 2012; White, 1981). Natural radiations in building materials related to external and internal

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Protein characterization and sequence analysis of ALLCE antimicrobial peptide from *Allium cepa*

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Abstract

Antimicrobial proteins/peptides produced by plant seeds participate in protection of seeds against pathogenic organisms. A study was carried out to investigate the *in silico* analysis of protein sequence localization, structure, homology modeling and 3D structure prediction of ALLCE-AMP in *Allium cepa*. Primary structure prediction and physico-chemical characterization were performed by computing theoretical isoelectric point (pI), molecular weight, total number of positive and negative residues, extinction coefficient, instability index, aliphatic index and grand average hydropathy (GRAVY). In the present study, homology modeling, a high quality of peptide 3D structure, was predicted by submitting the peptide sequence (target) to ESYPred3D web server. The template (1T12 chain A) was found to share 18.2% identity with the Query (B2CZN8). The model was validated using protein structure checking tools PROCHECK and ERRAT VALUE (62.353). The present study would be useful in studying protein-protein interactions and drug designing.

Key words

Allium cepa, ALLCE-AMP, PROCHECK, Structure prediction, Subcellular localization

Introduction

Plants have established numerous defense systems to guard themselved from invasion of pathogens during their evolution (Liu *et al.,* 2000). Plants produce secondary metabolites in the form of antimicrobial peptides or proteins showing vast variety in antimicrobial spectrum, structure, function and mechanism of action. Most interestingly, there is growing proof that AMPs also fulfil essential biological functions (Nikoletta and Florentine, 2013). Previous studies have shown that EtOH extract from fly maggots can potently inhibit MRSA and VRE strains, with a ready supply of inhibitory compound being recovered in separated butanol fraction (Sang *et al.,* 2010). AMPs are gene-encoded and are either constitutively expressed or quickly copied upon induction. In higher eukaryotes invading microbes and their products, e.g. lipopolysaccharides (Mendez-Samperio *et al.*, 2007; Amlie-Lefond *et al.,* 2005), or host cellular compounds, such as butyrate (Murakami *et al.*, 2002), vitamins (Schauber *et al.,* 2006) cytokines (Wolk *et al.*, 2004; Wilson *et al.*, 2007; Lai and Gallo, 2009) and encourage AMP manufacture. Studies of DNA and protein sequence homology are essential for variety of purposes and have consequently developed routine in computational molecular biology. The amino acid sequences and construction of Ace-amp1 protein have been determined which differs in few amino acid sequences to ALLCE antimicrobial peptide (ALLCE-AMP) from *Allium cepa*. AMPs function is strictly dependent on structural and physico-chemical properties to increase antimicrobial activity usually by changing molecular size and charge, residues arrangement, amphipathicity, hydrophobicity and helix folding probability (Tossi *et al.,* 2000; Tain *et al.,* 2009).

Allocating subcellular localization to protein is an important step towards interpreting its interaction partners,

INTERNATIONAL JOURNAL OF INNOVATIVE RESEARCH & DEVELOPMENT

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A Survey on Threshold Based Segmentation Technique in Image Processing

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Abstract
The present paper describes the study of the threshold techniques in image segmentation. Image segmentation is one of the fundamental approaches of the digital image processing. Image segmentation is used widely in many applications. Several general purpose algorithms and techniques have been developed for image segmentation. Segmentation applications are involving detection, recognition and measurement of features. The purpose of image segmentation is to partition an image into meaningful regions with respect to a particular application. Segmentation techniques can be classified as either contextual or non-contextual. Thresholding is a Non-Contextual Approach. This method is based on a threshold value to turn a gray-scale image into a binary image. In Histogram Dependent Technique, a histogram is computed from all of the pixels in the image and this paper enumerates and reviews a comparative performance of threshold technique as Histogram Dependent Technique (HDT) based on Global Threshold, Local Threshold and Adaptive Threshold one another

Keywords: Digital image processing, Image segmentation, Non-Contextual Approach threshold technique, Histogram Dependent Technique (HDT), adaptive threshold technique

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Kinetics and mechanism of oxidation of aminoalcohols with N-Bromopthalimide in aqueous acetic acid

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ABSTRACT

The kinetics of oxidation of amino alcohols (AA), viz., mono ethanolamine (MEA), di ethanolamine (DEA) and tri ethanolamine (TEA) by N-Bromo phthalimide (NBP) in the presence of mercuric acetate have been investigated in aqueous acetic acid medium. The order in [NBP] was found to be unity and fractional order dependence on [substrate] was observed. Michaelis -Menten type mechanism was proposed. Activation parameters have been evaluated.

Keywords: Kinetics, oxidation, amino alcohols, N-Bromopthalimide.

INTRODUCTION

Amino alcohols (AA) are organic bases containing amino and alcoholic functional groups, find extensive applications in the synthesis of surfactants, pharmaceuticals and as addition agents in metal finishing industries [1]. Kinetic results have been reported in literature for the oxidation of amino alcohols by various oxidizing agents[2-6].The N-halo compounds are known to act as sources of halonium ions and these compounds have been used as brominating [7]and oxidizing agents[8, 9]in synthetic organic chemistry as well as analytical reagents especially in acid medium. The N-halo compounds reaction with organic substrates such as anisole, alcohols and amines leads to the products of net oxidation followed by elimination of HBr. Though the oxidation of various organic and inorganic substrates by N-halo compounds has been investigated by several workers [10-13], kinetic study on the oxidation of amino alcohols by NBP is lacking. In view of the above; the present paper reports the studies on the kinetics of the NBP oxidation of ethanolamine, di ethanolamine and triethanolamine in aqueous acetic acid medium.

MATERIALS AND METHODS

The reagents employed were ethanolamine, di ethanolamine, tri ethanolamine (Merck) and N-Bromopthalimide (Sigma Aldrich). All the chemicals used were of analytical grade. Acetic acid was refluxed with chromic oxide and acetic anhydride for 6 h and then fractionally distilled according to literature procedures [14].The solution of NBP was always prepared freshly and was standardized iodometrically. All aqueous solutions were prepared in doubly distilled water.

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Employee Retention: A Strategic Tool for Organisation Profitability

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Abstract:
During disruptive periods of organizational changes, Organizations tend to retain star performers and other rainmakers for its profitability. Employees are the lifeline of an organization and contribute effectively to its successful running and profit making. The biggest challenge for organizations is to maintain a stable workforce by reducing employee turnover through better benefits and flexible workplace policies which makes results in significant cost savings. The present paper focuses on how employee retention can be a strategic tool for organization profitability.

Keywords*: Employee, Organization, Turnover, Retention, Profitability*

1. Introduction

Globally, organizations are facing multiple challenges around managing the complex issues of business performance. Organizations are relining their business to mitigate challenges and improve the business performance. In today's fast paced business environments where organizations are constantly striving to achieve business performance confronted by social developments such as globalization, technological improvements increasing global competition. These evolutions cause not only a shortage of workers, but also a risk of losing talented employees. This loss of talent increases the importance of retaining talent. Lockwood (2006, p. 2) describes talent as "... the vehicle to move the organization to where it wants to be". Accordingly, talent is becoming increasingly important and will continue to do so (Hiltrop, 1999). It therefore becomes increasingly important for organizations to retain talented and skilled employees in order to maintain their competitive advantage and improve the business performance. Losing such employees means a loss of investment in new employees to be hired and trained. Moreover, employees take their know-how with them and thus the company risks a potential loss of confidential information to competitors (Frank et al., 2004; Walker, 2001).

2. Employee Attrition

Georgy P. Smith shows businesses how to build productive and profitable work environments that attract, keep and motivate their work force he says "Transforming your workforce from high turnover to high retention"

Once an individual is employed in an organization he usually remains married to the organization till retirement. There was hardly any occasion when the employee quit by himself. In recent times, Job hopping has become a concern for technological environment in which the existing job becomes obsolete and opportunities becomes limited so employee don't like to stay in the same company for longer period of time. Their aim is to take advantage of the present market to overcome this situation it has become imperative for organizations to look in to the causes of this high turnover.

Surely, as more and more qualified people find themselves up for grabs by employee hungry corporate, companies feverishly trying to retain their own people by hook or by crook. The attrition is like an atom bomb being dropped on the economy. Companies invest lots of time and money in training and educating employees. These companies are severely affected when employees check out, especially in the middle of some big company project or venture. Although employees most often prefer to stay with the same company and use their time and experience for personal growth and development, they leave mainly because of work related stress and dissatisfactions. More and more companies have now realized the importance of a healthy work culture and have a gamut of people management good practices for employees to have that ideal fresh work-life.

The cost of employee turnover for businesses is high, regardless of the level of wages being paid to the departing or incoming employees. Workplace policies that improve employee retention can help companies reduce their turnover costs.

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King Saud University

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ORIGINAL ARTICLE

Evaluation of antibacterial activity of crude protein extracts from seeds of six different medical plants against standard bacterial strains

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KEYWORDS

Crude protein extracts;
Bacterial strains;
Antibacterial activity;
Agar well assay

Abstract A huge group of natural antimicrobial compounds are active against a large spectrum of bacterial strains causing infectious threat. The present study was conducted to investigate the crude extracts of antimicrobial protein and peptide efficacy from six medicinal plant seeds. Extraction was carried out in Sodium phosphate *citrate* buffer, and Sodium acetate buffer using different pH. Antimicrobial activities of these plants were determined by the microbiological technique using Agar well diffusion Assay. Extremely strong activity was observed in the seed extracts of *Allium ascolinicum* extracted in sodium phosphate citrate buffer at pH (5.8) against *Proteus vulgaris*, *Escherichia coli* and *Staphylococcus aureus* with zone of inhibition 17 mm, 17 mm and 15 mm and *Rumex vesicarius* at pH (7.6), *Ammi majus* at pH (6.8), *Cichorium intybus* at pH (7.4) and *Cucumis sativus* at pH (7.8) also showed better sensitivity against the bacterial strains with zone of inhibition ranges 16–10 mm and some of the strains were found to be resistant. Antibacterial activity pattern of different plant extracts prepared in sodium acetate buffer pH (6.5), among all the plant seed extracts used *Foeniculum vulgare* had shown good inhibition in all the bacterial strains used, with zone of inhibition ranges 11–12.5 mm, The extracts of *C. intybus* and *C. sativus* were found to be effective with zone of inhibition 11–6 mm and some of the strains were found to be resistant. Most of the strains found to have shown better sensitivity compared with the standard antibiotic Chloramphenicol (25 mcg). Our results showed that the plants used for our study are the richest source for anti-

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Table Of Content

IDENTIFICATION OF VACCINE TARGETS IN KLEBSIELLA PNEUMONIA USING VIOLIN

Author Name(s): *Swathi K, Swetha C, Uma sree G, Kavitha, Janardhan K

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Abstract

Klebsiella pneumoniae causes community acquired, nosocomial infections & other diseases like bacteremia, hepatic abscess, meningitis, respiratory & urinary tract infections worldwide. This organism is rod shaped, gram-negative, non-motile encapsulated, lactose fermenting facultative anaerobic bacterium, found as the normal flora on the mouth, skin and intestine. Klebsiella pneumoniae belonging to the Enterobacterceae family typically expresses 2 types of antigens –O antigen a component of Lipopolysaccharide & -K antigen a capsular polysaccharide. Many antibiotics are recommended for the treatment, but the organism is showing resistance making the treatment challenging. The solution could be use of vaccines; a polyvalent pneumococcal polysaccharide vaccine was licensed for the treatment of pneumococcal infections during late 1977, but there were reports of its failure. VIOLIN a web-based vaccine tool integrates vaccine literature data mining, vaccine research data curation & storage & curated vaccine data analysis for vaccines & vaccine candidates developed against various pathogens of high priority in public health & biological safety. VIOLIN also provides a program for vaccine target prediction. In our study we have used this tool for the detection of vaccine targets for K.pneumoniae NTUH-K2044 and it was found that the putative outer membrane can be synthesized in vivo and can be used as a potent protein sub-unit protein against Klebsiella infections.