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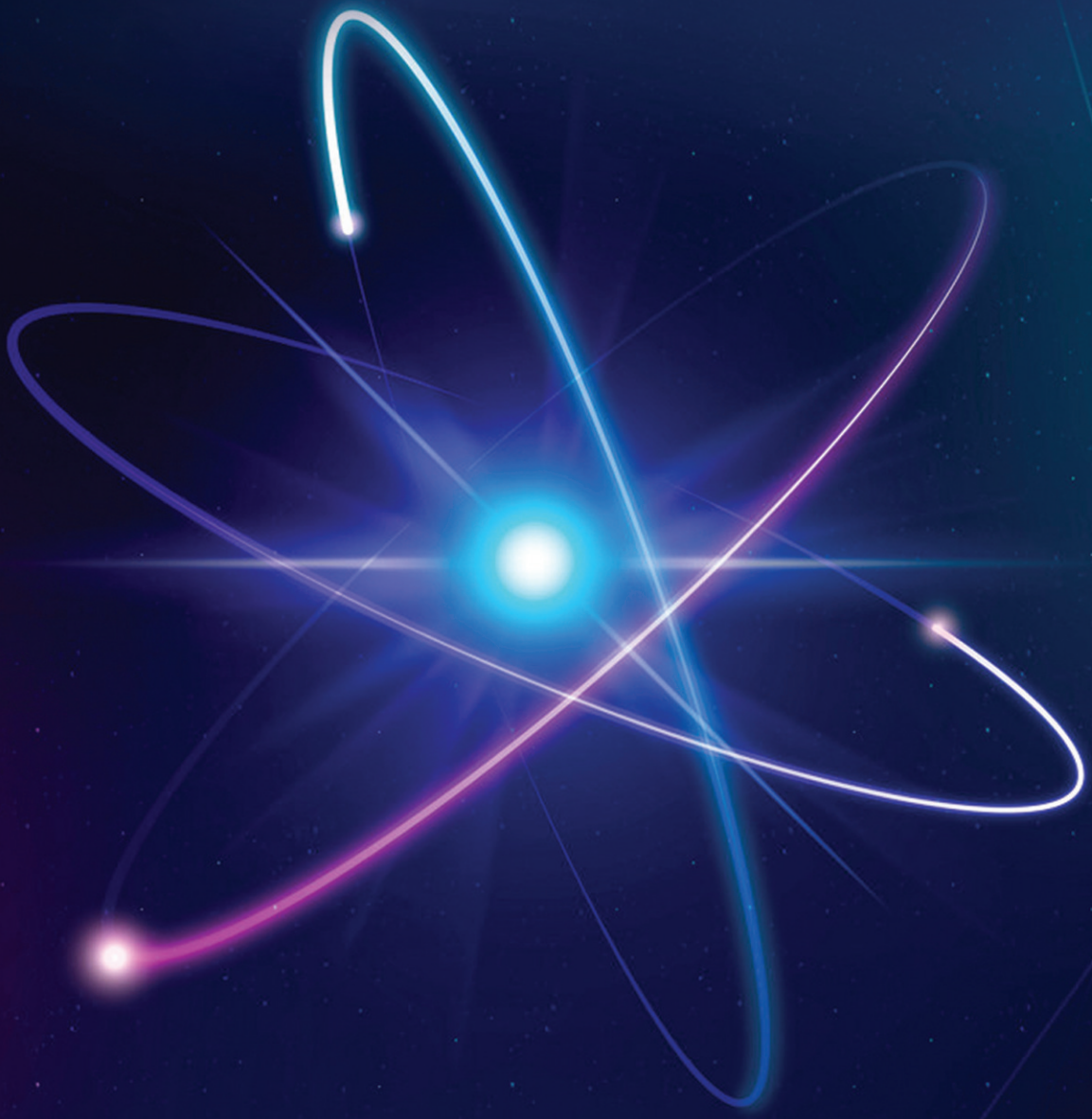

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STATUS OF NEEDLE FISH LANDING AND LENGTH SIZE RANGE OF *Tylosurus acus melanotous* FROM ANDROTH ISLAND LAKSHADWEEP

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ABSTRACT

The status of Belone fishery of Androth Island is discussed based on the data during the period of three years (June 2014 to May 2017). The annual needle fish landing of Androth Island was

120.102 tonnes (June 2014 - May 15), 131.294 tonnes (June 2015 - May 2016) and 114.352 tonnes (June 2016 - May 2017). The species landed in Androth is *Tylosurus acus melanotous* (88

%) *Tylosurus corcordilus* (11%), and *Ablennes hians* (1%). The month-wise gillnet effort varied from 50 to 384.The highest monthly CPUE (163) was recorded in the month of July, 2015 and lowest (11) in the month of September, 2014. The full beaks are mainly exploited in gill nets. Pablo boats of 5 to 8m overall length with inboard and outboard engines are engaged throughout the season for belone and hemiramphid fishery in Androth. The present study is the first estimate of species wise landing of needle fishes in Androth Island Lakshadweep.

Keywords: Fishery, Belone, CPUE, *T.corcordilus*, *T. acus melanotous* , *Ablennes hians* , Androth

INTRODUCTION

Lakshadweep Sea is rich in fishery resources like tuna, gar fishes, half beaks, sharks, bill fishes and reef fishes etc. and needle fishes are the very important domestic fishery. The major gear operation are pole and line, troll line, gillnets, and hook and line while the major crafts are Mechanized, Motorized and Non-mechanized country craft. Needlefishes are commonly known as full beaks and are considered to commercially important pelagic fishery resource in the view of good quality of meat. The gar fish is epipelagic and lives solitarily or small groups usually near surface. It feeds on small schooling fishes (Golani et al. 2006). Needlefishes are a small family of beloniform fishes (Rosen et al.1981 and Collette et al. 1984). Most of the needle fishes are marine but 12 species are fresh water. In India annual catches of full beak and half beaks increases from about 4069 tonnes in 2012 to around 4305 tonnes in 2013 (CMFRI 2014). Most of the landings are reported from Tamil Nadu region followed by Kerala.

Studies related to the assessment of marine fishery resource of Lakshadweep waters is very scanty. Androth is the major fishing area contributing about 50-60% of the total Belone

catch. Needle fishes are plenty in Lakshadweep waters, however there is no detailed information available on species wise landing in Lakshadweep. Even though needlefish fishery is the second largest fishery in Lakshadweep (Shahul et al., 2018) their current exploitation is low compared to tuna fishery. Therefore, present study deals with the status of Belone fishery of Androth Island.

MATERIALS AND METHODS

The study was conducted during June 2014 – May2017 in Androth. The Needle fish fishery conduct only half day fishing trip (6am – 12pm). We are followed the sampling design of CMFRI for estimating the fishery data. In this, observation of fish landing data, a month is divided into 3 groups, each of 10 days. From each group, a cluster of 6 consecutive days are selected systematically with a random start with a sampling interval of ten days. The first five days of a month, a day is selected randomly, which together with the next 5 consecutive days (6 days in all) form the first cluster. The next 6 days each from the other groups follow systematically. The average catch and species composition by weight for the observed units were multiplied by the number of units landed on the day to get the days catch. The total species-wise catch and effort on the observation days were raised to the month by multiplying it with the actual fishing days in the month. The total catch, catch per unit effort and seasonal distribution of the groups shall be studied. And also used questioners, Personal interviews for studying fishing methods.

RESULTS

Craft and gear

Wooden country crafts and some Pablo boats of 5 to 8m overall length with inboard and outboard engines are engaged throughout the season for belone and hemiramphid fishery in Androth Islands. The gear operated is a type of encircling gill net called chuttuballa / Muralbala. The mesh size varies from 30 to 60mm with depth of the net varying from 4.5 to 10m depending upon head rope length. Plastic floats or rounded thermocoles are used at regular intervals and foot ropes are connected with sinkers. For identifying shoals of half beaks and full beaks, a traditional method using brown colored coconut leaves have been employed. Fishes were jumped above these small pieces of coconut leaves, if present.

Fishery

Full beaks establish a very significant portion in the marine fish landings of Lakshadweep. The exact landing data of full beaks and half beaks are not available as many states of India have no separate landing data of belonids. This group might have been included under half beaks and full beaks together or under the miscellaneous category. The estimated half beaks and full beaks landings in India were 7316 tonnes in 2000, 4378 tonnes in 2001, 5922 tonnes in 2002 and 5649 tonnes in 2003, 4069 tonnes in 2012, 4305 tonnes in 2013 respectively (CMFRI 2002; 2013). Kasim et al. (1996) estimated that Tamil Nadu, Kerala and Lakshadweep contributed 42.6, 25.6 and 2.6 percent respectively of the total landings of full beaks and half beaks.

The annual needle fish landing of Androth Island was 120.102 tonnes (June 2014 - May 15),

131.294 tonnes (June 2015 - May 2016) and 114.352 tonnes (June 2016 - May 2017). During the first, second and third year the month wise landing of needle fish showed high landing in April (31.99T), June (30.99 T) and January (20.95 T) and the lowest in September (2.01 T), April (1.47T) and June (3.65 T) respectively (Fig: I).

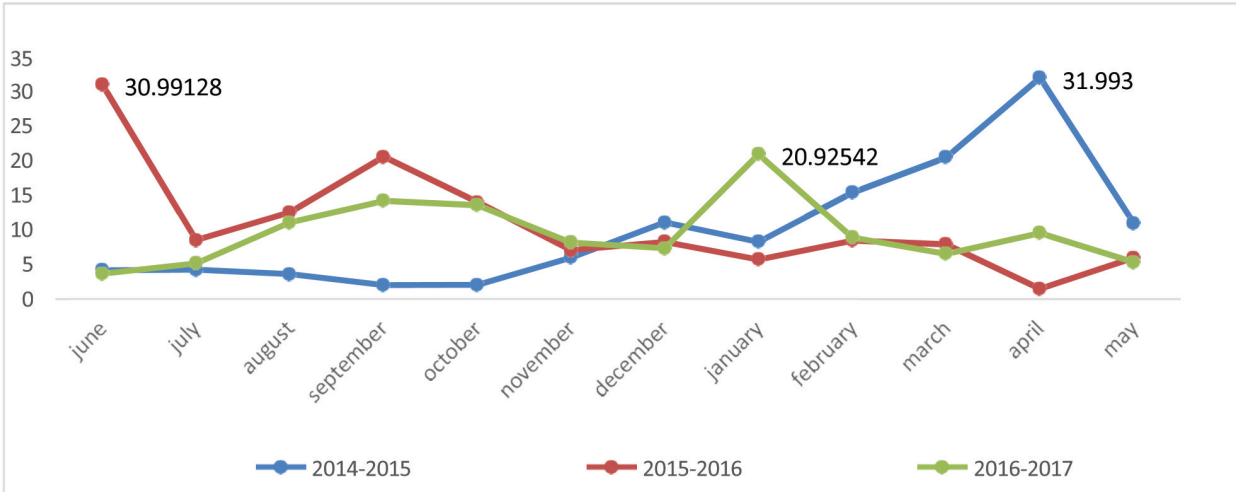

Fig: I. Total annual catch of belonids at Androth during the period of June 2014-May 2017 (Tonnes)

The month-wise gillnet effort varied from 50 to 384 units with an average of 170 units (FIG: II). The highest monthly CPUE (163) was recorded in the month of July, 2015 and lowest (11) in the month of September, 2014 (FIG: II). The catch indicate that the fishes were landed throughout the year.

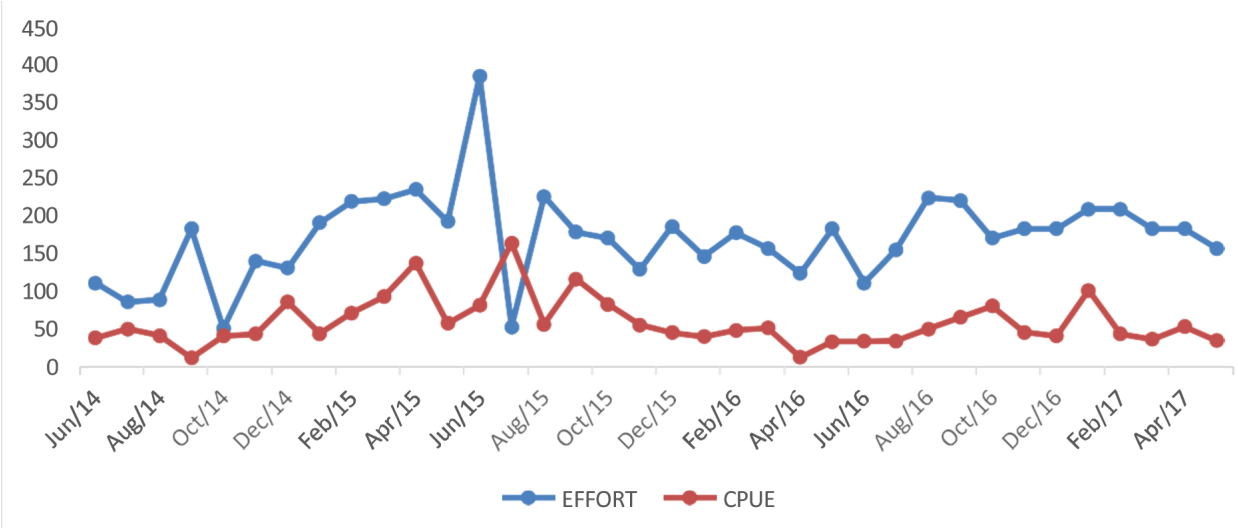

Fig: II. Effort and Catch per unit effort of belonids at Androth during the period June 2014- May 2017

Species composition

In Androth Island three Species of full beaks *T. corcodilus* (Peron & Le Sueur), *T. a .melanotous* (Bleeker), *A. hians* (Valenciennes) supported the fishery. *T. a. melanotous* was the dominating species among the full beaks contributing 88% through the years followed by *T.corcordilus* (11%) and *A.hians* (1%) Fig: III.

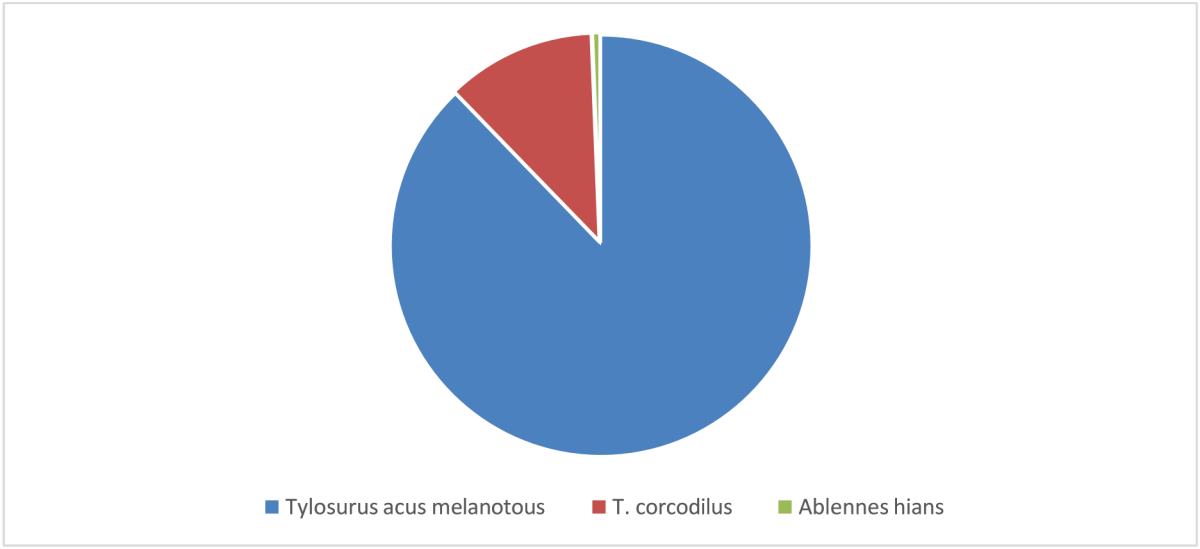

Fig:III. Species composition of belonids at Androth during the period of June 2014- May 2017T

The length range of *T. acus melanotus* varied form 22-84 cm (mean size 58.6cm). The highest landing size was 76-84 cm followed by 76-78cm. Length which 28% of this species was vulnerable to gear.

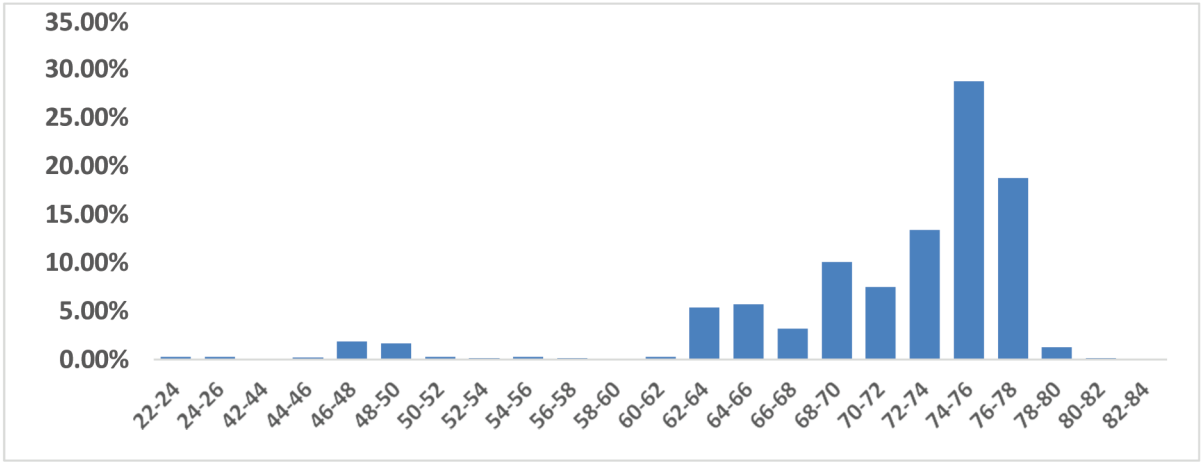

Fig:IV . Length frequency of belonids at Androth during the period of June 2014- May 2017

DISCUSSION

The gar fish is epipelagic and lives solitarily or small groups usually near surface it is feed on small schooling fishes (Golani et al 2006). Needle fishes are small family of beloniforms fishes (Rosen et al .1981 and Collette et al. 1984) and most of the needle fishes are marine. Jones and Kumaran (1980) reported six species of needlefish from Lakshadweep and only three species ie.,

A. hians, T. a. melanotus and *T. crocodilus* constitute the regular fishery of the region (Shahul Hameed et al. 2018).The largest contributing species is *T. a. melanotous* and mainly exploited using gill nets. Kasim, et al., (1996) reported that in Tuticorion region *A.hians* was the major sharing, but in no data in *T. a. melanotous*. Liao and Chang (2011) reported that size at first maturity of *T. a. melanotous* was 50.6 and 46.4 cm total length for female and male respectively, ie 74-76 cm (mean size – 58.6cm TL) indicating the majority of the fish might mature and spawn at list once before being caught.

We conclude that the needle fish species of Androth Island have healthy stock as reported in earlier study (Shahul Hameed et al. 2018). Mainly gillnet, drift gillnets and purse - seiners are used for exploitation of full beaks (Liao and Chang, 2011; Kasim et al. 1996; Tulin Cokeret et al. 2013; Chaari, 2016) and very small quantities in Troll line and Hook and line in Lakshadweep. The Present study is the first estimate of species wise landing of needle fishes in Androth Island Lakshadweep. For better understanding for fish stocks and their sustainable utilization, additional studies on population dynamics and reproductive biology of individual stocks is highly recommended. This will help in better understanding and management of fish stocks.

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DIVERSITY OF CORAL REEF FISHES OF AMINI ISLAND, LAKSHADWEEP ARCHIPELAGO

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ABSTRACT

The present study recorded the diversity of coral reef fishes from the Amini Island of Lakshadweep archipelago during 2019-2020 period, using different gears such as baited trap, cast net, and seine net. This study documented eighty-four species of fishes belonging to twenty- eight families, of which two species were listed under the IUCN Red list. Among the 28 families, two families such as Acanthuridae and Labridae are the species-rich families (11 species each). This study revealed the high diversity of coral reef fishes on Amini Island and showed the importance of the need for ecosystem conservation.

Keywords- Lakshadweep, Amini Island, Coral reefs, Diversity, Fishes.

INTRODUCTION

India is one of the 17 mega-biodiversity countries harbouring a variety of species-rich ecosystems including marine habitats (Ajith Kumar *et al.,* 2012). It has a coastline of more than 800 km, with an Exclusive Economic Zone (EEZ) of 2.02 million km^2 and a continental shelf area of 4,68,000 km^2 (Ajith Kumar *et al.,* 2012). The coral reef areas spread across the mainland and the islands of Andaman & Nicobar and Lakshadweep. There are four major coral reef regions in India such as the Gulf of Mannar, the Gulf of Kutch, the Andaman & Nicobar islands and Lakshadweep. The lagoons and reef flats in the Lakshadweep group of islands are the richest both in regard to the number of species and their numerical abundance (Murty *et al.* 1989; Vijayanand and Vargheese, 1990.)

The union territory of Lakshadweep is an archipelago situated in the Arabian sea between 80^0 00' N and 12^0 30' N latitude and 71^0 00' E and 74^0 00' E longitude. The length of the coastline is 132 km. which is approximately 1.6% of Indian's total coastline. The islands have a lagoon area of around 4000 km^2, territorial waters cover with 20000 km^2, continental shelf of 4000 km^2, and an Exclusive Economic Zone (EEZ) of 0.4 million km^2. It is the largest atoll system in the world with 12 atolls (Jones,1986). The islands consist of coral formations built on submarine ridges (Laccadive-Chagos ridge) steeply from a depth of about 1500 m to 4000 m off the west coast of the mainland of India (Jones, 1986). These islands are formed by the accumulation of coral sand in the form of sand bars with the action of wind, waves and currents.

Lakshadweep is known for its rich marine ecosystem. This consists of coral reefs, sea-grass, and diverse organisms including diverse types of fishes. The lagoons and reef flats of the Lakshadweep are rich in corals represented by 104 species belonging to 37 genera (Pillai *et al.*, 1989). About 78 species of echinoderms are also reported from these islands (James, 1989). Thomas (1989) reported 91 species of sponges from the region. Kaliaperumal *et al.*, (1989) reported 114 species of seaweeds and 6 species of seagrasses from the region. Moreover, there are wide ranges of other invertebrate fauna like ornamental and edible molluscs, the hermit crabs known from the

lagoons (Appukuttan *et al.*, 1989). This abundance and diversity of flora and fauna in the lagoon offer a wide variety of habitats for a multiplicity in the range of fishes which are smaller in length, brightly coloured and well-suited for aquarium purposes, offering great potential for developing a fishery for these fishes which have great demand in the export market as live fishes. Murty *et al.*, (1989) reported 138 species of ornamental fishes (reef fishes) belonging to 33 families from the Lakshadweep. Murty (2002) Jones and Kumaran (1980) published a comprehensive account describing 603 fishes from Lakshadweep. Sixteen more species were added by Venkateswarlu and Ilango (1982) to the ichthyofauna of Lakshadweep. In addition, Balachandran and Nizar (1989) included three more species to the list. In 1991, Rao documented 740 fishes from Lakshadweep archipelago.

The present study was conducted on Amini Island of Lakshadweep. Amini island is at a distance of 407 km (220 nautical miles) from Kochi and is located between Kavaratti Island in the south and Kadmat island in the north. This island has an oval shape with a width of 1.20 km at the broadest point and a length of 2.70 km. It lies between 11° 06' and 11° 08' N latitude and 72° 42' and 72° 45' E longitude, having a land area of 2.60 sq. km and a lagoon area of 1.50 sq. km. The island is 2-3 m above the mean sea level, with a depression at the centre. There are 37 species of corals under 15 genera in Amini island (Pillai and Jasmine., 1989). Murty (2002),

observed eight families in Amini island. Suresh (1997), reported 57 species of fishes belonging to 19 families from Amini Island and argued that Amini island is rich in Labrid fishes (wrasses) (over 80% of the total population in the lagoon) particularly in the intertidal region along the eastern side. However, Murty (2002), focused on fishes having ornamental value.

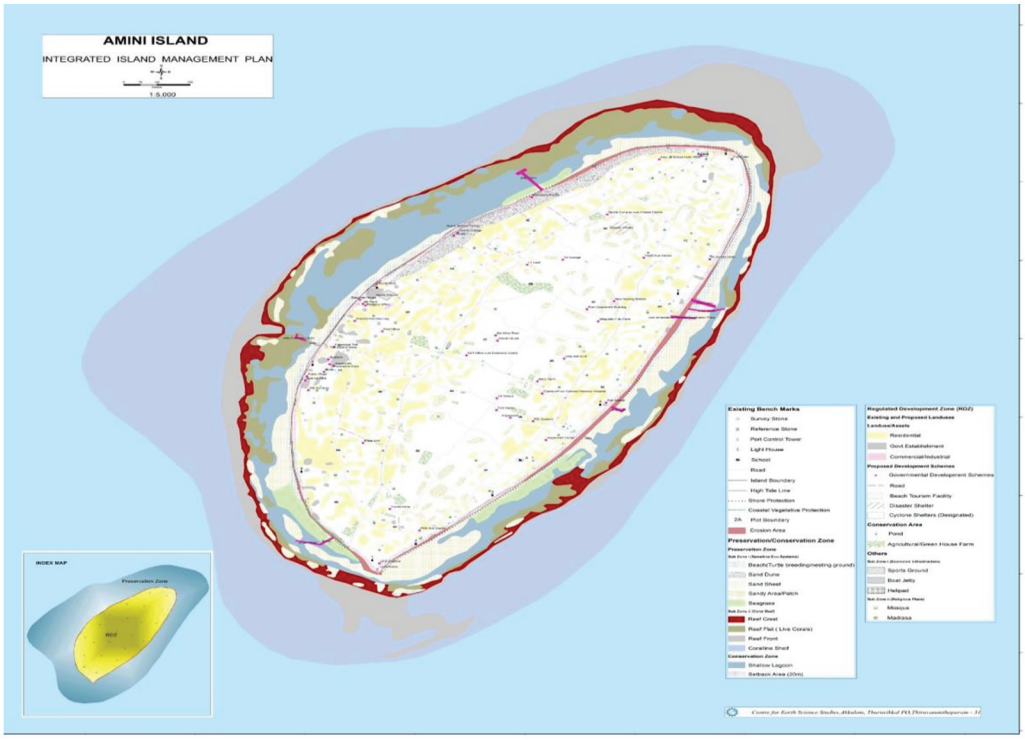
In the present scenario, the fragile ecosystem of Lakshadweep falls into severe changes. This includes death of corals due to bleaching and other unfavourable changes in sea and massive destruction in the sea-grass bed. Moreover, anthropogenic activities in the intertidal area also affect the ecosystem of Lakshadweep. Thus, this work was carried out with the aim of understanding the current status of the ichthyofauna of Lakshadweep with special reference to Amini island. So far studies have been taken the case of Lakshadweep in its entirety, hence this study narrow it down to Amini island.

METHODOLOGY

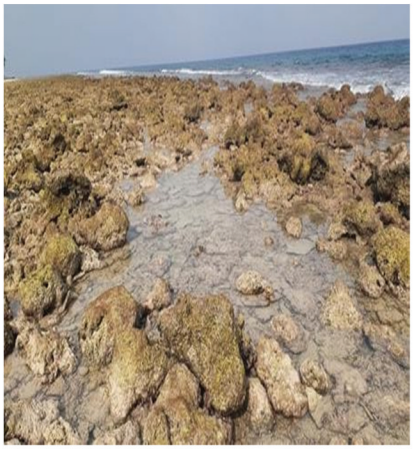
The methodology employee's quantitative study is based on the data collected from Amini Island. Data were collected on seasonal basis from September 2019 to August 2020, . Fishes were captured at the beginning of low tide and the beginning of high tide (intertidal condition) for the ease of locating fishes. Reef fishes were caught by using different gears. Baited-trap (**BT**), Cast net (**CN**) and Seine net (**SN**) are used. The net was operated by three or four people. The net was placed vertically in the water by two people, the other persons scare the fish school/shoal and drive them into the vertically held net. After encircling the school/shoal, the net was hauled up. Fishes identified by local names, and numbers were counted and noted in the datasheet.

However, Fishes were processed for a thorough cleaning, immediately after capturing them. The fins were spread and specimens were placed on a clean flat surface. The photographs of the species were collected through the mobile phone. The photographs were taken in lateral view, for the identification of fishes. The identification of coral fishes was prepared on the basis of photographs and with the help of scientists of the biodiversity wing of CMFRI. The colour of the fish, the shape and position of the mouth, shape and size of the fins were some of the morphological characteristics used for primary identification.

Picture: 1. Map of Amini Island



Picture 2 & 3 Showing different views of collection sites during low-tide



Picture :1

Picture :2

RESULTS

This study documented a total of 84 species of reef/ reef-associated fishes coming under 28 families. Among these; some members of families, Pomacentridae, Carangidae, Scaridae, Pempheridae, Chaetodontidae and Caesionidae could be observed during all three collections from this island. Families of wrasses (Labridae), surgeon fishes and unicorn fishes (Acanthuridae) were the most abundant. They were followed by Serranidae, Carangidae, Lutjanidae, Mullidae, and Pomacentridae. *Anampses* sp. in the Labridae family was the predominant coral fish species on Amini island. Diodontidae, Tetraodontidae, Fistularidae, Sphyraeniddae, Synaceiidae, Kyphosidae, Pempheridae, Haemulidae, Pinguipedidae, Mugilidae were the least abundant families. Bigeye barracuda, *Sphyraena forsteri* Cuvier of the family Sphyraeniddae and red cornet fish, *Fistularia petimba* Jordan and Seale of the family Fistularidae were rarely seen in the catches from the lagoon of Amini Island.

After the first collection, (post-monsoon) around 79 species of fishes were obtained of which 26 species were coming under the category of solitary fishes and the rest of 53 species were gregarious. During the second collection, (winter) a total of 56 species were obtained of which 15 were solitary and 41 were gregarious. The third sample collection (pre-monsoon) resulted in a total of 52 species of which 13 species were solitary and 39 were gregarious in nature.

Out of the collected 84 samples of fish species, **2 were scheduled in the Red list** of the International Union for the Conservation of Nature and Natural Resources **(IUCN)**. Arabian carpet shark, *Chiloscyllium arabicum* (Gubanov), is in the category of "Near threatened species" (NT) within the IUCN scheduled red list. The dusky grouper, *Epinephelus marginatus* (Lowe) is the Vulnerable Species (VU) stated as per the report of IUCN. Though, the levels of fishing in the islands are very small scale, the fishermen and public need to be made aware of the state of the species'.

Picture 4: Arabian carpet shark (***Chiloscyllium arabicum*** Gubanov)

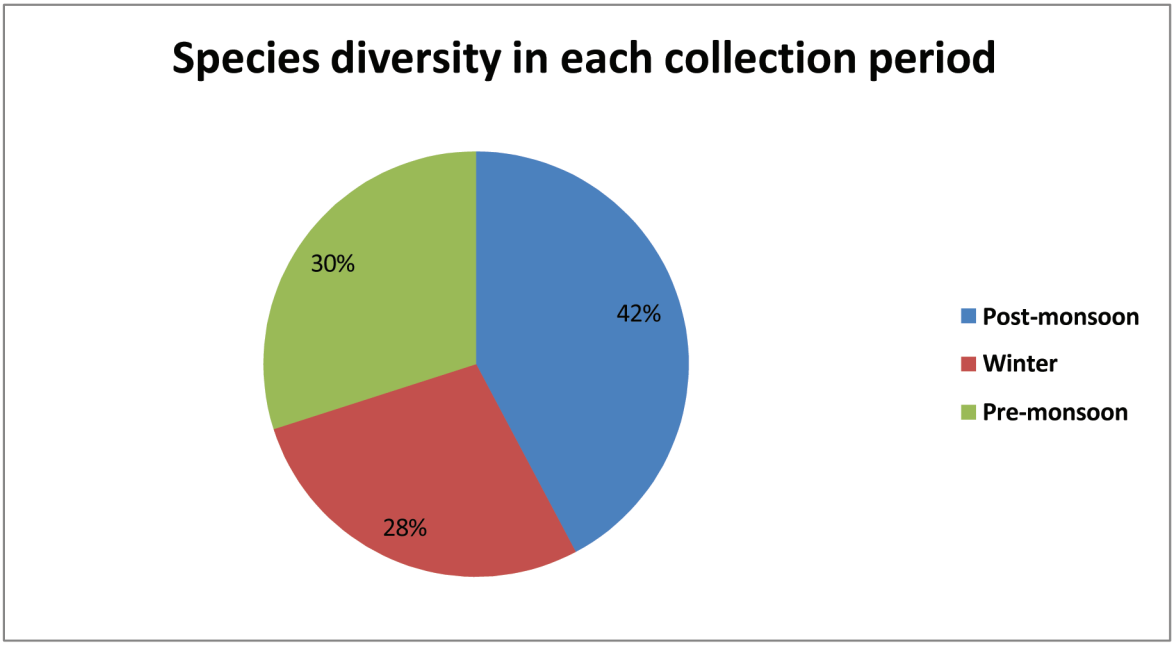
Table. 1: Species diversity of Coral-fishes belonging to different families in Amini island, Lakshadweep

Sl. No.	FAMILY	SPECIES
I	Hemiscyllidae	*Chiliscyllium arabicum*
II	Muraenidae	*Gymnothorax undulates*
III	Synanciidae	*Synaceia verrucosa*
IV	Mugilidae	*Chelon parsia*
V	Hemiramphidae	*Rhynchorhamphus malabaricus*
		Hyporamphus dussumieri
VI	Belonidae	*Tylosurus crocodilus*
VII	Holocentridae	*Myripristis seychellensis*
		Myripristis berndti
		Sargocentron macrosquamis
VIII	Pomacentridae	*Abudefduf sordidus*
		Abudefduf saxatilis
		Abudefduf vaigiensis
		Chrysiptera biocellatus
		Chrysiptera sp.
IX	Carangidae	*Caranx ignobilis*
		Giant trevally
		Trachinotus baillonii
		Trachinotus sp.
		Decapterus russelli
		Caranx sexfasciatus
		Elegatis bipinnulata
X	Sphyraeniddae	*Sphyraena forsteri*
XI	Fistularidae	*Fistularia petimba*
XII	Pinguipedidae	*Parapercis millipunctata*
XIII	Labridae	*Thalassoma Hardwicke*
		Thalassoma jansenii
		Halichoeres scapularis
		Stethojulis balteata
		Anampses sp.
		Halichoeres hortulanus
		Coris Formosa
		Stethojulis trilineatus

		Anampses caeruleopunctatus
		Halichoeres melas
		Novaculichthys taeniorus
XIV	Scaridae	*Scarus frenatus*
		Scarus viridifucatus
		Chlororus sp.
XV	Mullidae	*Parupeneus barberinus*
		Upeneus quadrilineatus
		Parupeneus trifasciatus
		Parupeneus macronemus
		Mulloidichthys flavolineatus
XVI	Pempheridae	*Pempheris vanicolensis*
XVII	Kyphosidae	*Kyphosus vaigiensis*
XVIII	Serranidae	*Cephalopholis argus*
		Variola louti
		Epinephelus marginatus
		Aetheloperca rogaa
		Epinephelus fasciatus
		Epinephelus macrospilos
		Epinephelus longispinis
		Epinephelus spilotoceps
XIX	Chaetodontidae	*Chaetodon citrinellus*
		Chaetodon auriga
XX	Haemulidae	*Plectorhinchus gibbosus*
XXI	Lutjanidae	*Lutjanus kasmira*
		Lutjanus fulviflemma
		Lutjanus bohar
		Lutjanus rivulatus
		Lutjanus gibbus
XXII	Caesionidae	*Caesio varilineata*
		Caesio xanthonota
		Dipterygonotus balteatus
XXIII	Siganidae	*Siganus lineatus*
		Siganus canaliculatus
XXIV	Acanthuridae	*Acanthurus lineatus*
		Acanthurus dussumieri

		Acanthurus gahhm
		Acanthurus triostegus
		Acanthurus mata
		Naso elegans
		Naso tuberosus
		Naso brevirostris
		Naso vlamingii
		Naso unicornis
		Acanthurus xanthopterus
XXV	Monacanthidae	*Cantherinus* sp.
XXVI	Balistidae	*Rhinecanthus aculeatus*
		Pseudobalistes flavimarginatus
		Melichthys niger
XXVII	Tetradontidae	*Canthigaster solandri*
XXVIII	Diodontidae	*Diodon hystrix*

Figure 1: Pie Diagram of Species Diversity in each collection period in Amini island.



The diagram reveals that, during the post-monsoon period, number of species is comparatively higher than the winter and pre-monsoon period. The species diversity was found to be low in the pre-monsoon season.

Picture 5: Dusky grouper (***Epinephelus marginatus*** Lowe)

DISCUSSION

The present study shows that 28 families occurred on Amini Island. Among these, Wrasses (Labridae), Surgeon fishes, and Unicorn fishes (Acanthuridae) are the most abundant. They were followed by Serranidae, Carangidae, Lutjanidae, Mullidae, and Pomacentridae. According to Murty *et al.* (1986), Labridae is the most abundant family in Amini followed by Mullidae, Pomacentridae, Acanthuridae, and Scaridae. The present work could record 20 more families from Amini island as against only 8 observed by Murty (2002). However, Murty (2002) targeted only fishes of ornamental value. Jones and Kumaran (1980) recorded that Acanthuridae and Labridae are the most dominant families in Lakshadweep Island. Suresh (1997) reported 57 species of fishes belonging to 19 families from Amini island. Whereas, this study finds that diversity of coral and coral-associated fishes in Amini island shows 84 species belonging to 28 families. Therefore, Amini Island is having a wide variety of coral-and coral-associated fishes that evolved over a period of time.

CONCLUSION

Eighty-four species of fishes under 28 families were recorded from Amini island among which ***Chiloscyllium arabicum Gubanov*** and ***Epinephelus marginatus Lowe*** are listed in IUCN Red list. Diversity and abundance of fishes were considerably different in various collections carried out over different time/season. The first sampling carried out during September yielded maximum species diversity and

abundance in the study site over the other two samplings (December and May). Rough weather of monsoon provides the lagoon a respite from fishing and other recreational use facilitating fishes to migrate to the lagoon in large numbers. Hence, generally, fish production from such places will be increased during the post-monsoon time. This study revealed the high diversity of coral reef fishes on Amini Island and showed the importance of the need for ecosystem conservation.

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FERMATEAN FUZZY SOFT ROUGH SETS AND ITS APPLICATION IN DECISION MAKING

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ABSTRACT

Rough set theory is an extension of set theory to study the data with incomplete information. Fuzzy set theory is an another tool to deal uncertainity which is different from rough set theory. Soft set theory is a relatively new approach to discuss vagueness. These three theories are mathematical tools for dealing with uncertainties and are closely related and can be combined in a truthful way. In this paper a discussion of the combinations of fermatean fuzzy set, rough set and soft set are done. It aims to introduce two new notions that are soft rough fermatean fuzzy set and fermatean fuzzy soft rough sets. Examples for both soft rough fermatean fuzzy set and fermatean fuzzy soft rough sets is provided to illustrate the developed approach.

Keywords: Soft set, rough set, Fermatean fuzzy set, Fermatean fuzzy soft rough set, Pythagorean fuzzy set, Pythagorean fuzzy soft rough set,

INTRODUCTION

Many well-known theories have been introduced for exploration of uncertainties in last few years to deal with the complicated models in engineering, economics, medical sciences, social sciences. Out of these theories, fuzzy set theory (L A Zadeh, 1965), soft set theory (Molodtsov, 1999), rough set theory (Pawlak, 1982) are the most popular theories.

Theory of Rough sets was an extension of the set theory to study the data with incomplete information. In rough set theory a subset of the universe is described by two approximations, called lower and upper approximations. The lower approximation of a set is the union of all equivalence classes contained in the set, whereas the upper approximation is the union of those classes which have non empty intersection with the set. Equivalence classes are the basic building blocks in rough set theory, for upper and lower approximations. A partition of a set induces an equivalence relation and vice versa. Therefore, we can view the properties of a rough set either by the partition of the set or by the equivalence relation.

The soft set theory offers a general mathematical tool for dealing with uncertain, fuzzy, not clearly defined objects. This theory is a relatively new approach to discuss vagueness.

In soft set theory membership is decided by adequate parameters, rough set theory deals with equivalence classes, whereas fuzzy set theory depends upon grade of membership. Although three theories are quite distinct yet deal with vagueness. Joint application of these theories may result in a fruitful way. There exist many complications in soft set theory mentioned in (Molodtsov, 1999). To overcome these

complications the new approach of SS was originated by Molodtsove, which is different from the other existing theories due to its parameterization tools. Soft set theory handles the vague and uncertain knowledge easily and it is free from the inherent complications. Due to these characteristics, the theory of Soft Set is famous among scholars in the recent era. In the recent scenario, Soft Set theory is one of the most significant areas of research. Maji (Maji et al., 2003) introduced various operations on Soft Sets. Through these operations, the theoretical study of Soft Set becomes improved and emerges very rapidly in research area. on the basis of (Maji et al., 2003) , (Ali et al., 2009) improved the existing literature and introduced some new operations on soft sets. They developed the concept of complement and asserted that certain De Morgans's laws are satisfied on the basis of these newly developed operations on Soft Sets. The generalization of Soft Set is improving very rapidly in the research area to hybridize the different mathematical structures with Soft Set. The combined structure of fuzzy set, soft set and rough set were presented by (Irfan Ali, 2011)

A fuzzy set is a class of objects with continuum of grade of membership. Such a set is characterized by membership (characteristic) function which assigns to each object a grade of membership ranging between zero and one.

Intuitionistic fuzzy set (Atanassov K T, 1986) consist of two functions which are the generalization of fuzzy set and like a fuzzy set, these two functions also map on unit closed interval. Here, the first function represents the membership grade and the second function represents non-membership grade. Intuitionistic fuzzy set set has a limitation that is the sum of both these functions does not exceed 1. Intuitionistic fuzzy set set plays a vital role for tackling vagueness and uncertainty. Many authors developed the new notions by combining rough set and Soft sets with Intuitionistic fuzzy set set and proposed the new results.

Yager (Yager, 2013) introduced Pythagorean fuzzy set, the square sum of membership and non- membership grades must not exceed 1, which got more attention of scholars in the recent era. (Hussain et al., 2019)proposed the concept of rough Pythagorean fuzzy ideals in semigroups. (Hussain et al., 2020) introduced the concepts of soft rough Pythagorean fuzzy set (SRPFS) and Pythagorean fuzzy soft rough set (PFSRS)

(Senapati & Yager, 2020) proposed Fermatean fuzzy sets (FFS), the cube sum of membership and non- membership grades must not exceed 1. He compared Fermatean fuzzy sets with Pythagorean fuzzy sets and intuitionistic fuzzy sets. (Muhammed, 2022) proposed the concept of rough Fermatean fuzzy ideals in semigroups. By viewing existing literature, it is clear that there does not exist any concepts of soft rough Fermatian fuzzy set (SRFFS) and Fermatian fuzzy soft rough set (FFSRS).

PRELIMINARIES

This section consists of a brief review of Intuitionistic fuzzy set(IF set), Fermatean fuzzy set (FFS), rough soft set (RSS), soft set(SS) and soft rough set.

Definition 2.1 (Atanassov K T, 1986)

For a universal set U, an IF set on U is denoted and defined as

$$\mathsf{f}_F = \{(k, \mu_{I_F}, \psi_{I_F}) |\ k \in U\}$$

Where $\mu_{\mathsf{f}_F}: U \to [0,1]$ represents the membership degree and $\psi_{\mathsf{f}_F}: U \to [0,1]$ represents non membership degree of $k \in U$ to the set f_F satisfying $0 \leq \mu_{I_F} + \psi_{I_F} \leq 1$.

Also $\pi_{\mathsf{f}_F}(k) = 1 - \mu_{\mathsf{f}_F} + \psi_{\mathsf{f}_F}$ is known as indeterminacy or hesitancy.

Definition 2.2 (Yager, 2013)

Let U be the universal set. A fermatean fuzzy set on U is denoted and defined as

$$\mathcal{F}_{\mathcal{F}} = \{(k, \mu_{\mathcal{F}_{\mathcal{F}}}, \psi_{\mathcal{F}_{\mathcal{F}}}) |\ k \in U\}$$

Where $\mu_{\mathcal{F}_{\mathcal{F}}}: U \to [0,1]$ represents the membership degree and $\psi_{\mathcal{F}_{\mathcal{F}}}: U \to [0,1]$ represents non membership degree of $k \in U$ to the set $\mathcal{F}_{\mathcal{F}}$ satisfying $0 \leq \mu^3_{\mathcal{F}_{\mathcal{F}}} + \psi^3_{\mathcal{F}_{\mathcal{F}}} \leq 1$.

Also $\pi_{\mathcal{F}_{\mathcal{F}}}(k) = \sqrt{1 - (\mu^3_{\mathcal{F}_{\mathcal{F}}} + \psi^3_{\mathcal{F}_{\mathcal{F}}})}$ is known as indeterminacy or hesitancy.

Basic operations union, intersection, complement on fermatean fuzzy sets are defined by (Senapati & Yager, 2020) and are given as

Consider two fermatean fuzzy sets

$$\mathcal{F}_{\mathcal{F}1} = \{(k, \mu_{\mathcal{F}_{\mathcal{F}1}}, \psi_{\mathcal{F}_{\mathcal{F}1}}) | k \in U\}$$

and

$$\mathcal{F}_{\mathcal{F}_2} = \{(k, \mu_{\mathcal{F}_{\mathcal{F}2}}, \psi_{\mathcal{F}_{\mathcal{F}2}}) | k \in U\}$$

$$\mathcal{F}_{\mathcal{F}1} \cup \mathcal{F}_{\mathcal{F}2} = \{(k, max\ (\mu_{\mathcal{F}_{\mathcal{F}1}}, \mu_{\mathcal{F}_{\mathcal{F}2}}), min(\psi_{\mathcal{F}_{\mathcal{F}1}}, \psi_{\mathcal{F}_{\mathcal{F}2}}) |\ k \in U\}$$

$$\mathcal{F}_{\mathcal{F}1} \cap \mathcal{F}_{\mathcal{F}2} = \{(k, min\ (\mu_{\mathcal{F}_{\mathcal{F}1}}, \mu_{\mathcal{F}_{\mathcal{F}2}}), max(\psi_{\mathcal{F}_{\mathcal{F}1}}, \psi_{\mathcal{F}_{\mathcal{F}2}}) |\ k \in U\}$$

$$\mathcal{F}_{\mathcal{F}}^{c} = \{(k, \psi_{\mathcal{F}_{\mathcal{F}}}, \mu_{\mathcal{F}_{\mathcal{F}}}) | k \in U\}$$

Definition 2.3 (Molodtsov, 1999)

Let U be a universal set and E be the initial set of parameters. Suppose that a function $F: E \rightarrow P(U)$, then the pair (F, E) is known to be a soft set on U, where $P(U)$ represents family of all subsets of U.

Definition 2.4 (Cagman N, 2010)

Consider a soft set (F, E) on U, then a relation Ω from $U \times E$ is known to be a crisp soft relation from a set U to E and is given as $\Omega = \{< (k, x), \mu_{\Omega}(k, x) > | (k, x) \in U \times E\}$

Where $\mu_{\Omega}: U \times E \rightarrow [0,1]$ and $\mu_{\Omega}(k, x) = \begin{cases} 1, & (k, x) \in \Omega \\ 0, & (k, x) \notin \Omega \end{cases}$

Definition 2.5 (Maji PK, Biswas R, 2001)

Let U be a universal set and E be the initial set of parameters. Suppose that a function $F: E \rightarrow P(U)$, then the pair (F, E) is known to be a fuzzy soft set on U, where $P(U)$ represents family of all fuzzy subsets of U.

Definition 2.6 (Cagman N, 2010)

Consider a fuzzy soft set (F, E) on U, then a relation Ω from $U \times E$ is known to be a fuzzy soft relation from a set U to E and is given as

$$\Omega = \{< (k, x), \mu_{\Omega}(k, x) > | (k, x) \in U \times E\}$$

Where $\mu_{\Omega}: U \times E \rightarrow [0,1]$ and $\mu_{\Omega}(k, x) = \mu_{F(x)}(k)$

Definition 2.7 (YY., 1998; YY, 1998)**:**

Consider a universal set U and $\Omega \subsetneq U \times U$ be a crisp relation. Consider the mapping $\Omega^*: U \rightarrow P(U)$ defined by $\Omega^*(k) = \{x \in U | (k, x) \in \Omega\}$. Then (u, Ω) is said to be an approximation space. Consider a nonempty subset $F \subsetneq U$, then the lower and upper approximations of F with respect to (u, Ω) are denoted by $\underline{\Omega}$(F) and $\bar{\Omega}(F)$ are defined as follows

$$\underline{\Omega}(F) = \{k \in U | \Omega^*(k) \subsetneq F\}$$

$$\bar{\Omega}(F) = \{k \in U | \Omega^*(k) \cap U \neq \phi\}$$

Then the pair $(\underline{\Omega}(F), \bar{\Omega}(F))$ is the crisp soft rough set where $\underline{\Omega}(F) \neq \bar{\Omega}(F)$.

1. Soft rough Fermatean fuzzy set (SRFFS)

In this section we will present the concept of SRFFS by combining the crip soft relation from U to E with the soft rough fermatean fuzzy approximation.

First we are discussing the soft rough fermatean fuzzy approximation operators.

Definition 3.1

Consider a crisp soft approximation space (U, E, Ω).

Let $\mathcal{F}_{\mathcal{F}} = \{(k, \mu_{\mathcal{F}_{\mathcal{F}}}(k), \psi_{\mathcal{F}_{\mathcal{F}}}(k)) \mid k \in E\}$, where $\mathcal{F}_{\mathcal{F}}$ is the fermatean fuzzy set.

Then the lower and upper soft approximations of F with respect to (U, E, Ω) are represented by $\underline{\Omega}(F_F) and \bar{\Omega}(F_F)$ and are defined as

$$\underline{\Omega}(F_F) = \{ (k, \mu_{\underline{\Omega}(F_F)}(k), \psi_{\underline{\Omega}(F_F)}(k)) \mid k \in U\}$$

$$\bar{\Omega}(F_F) = \{ (k, \mu_{\bar{\Omega}F_F)}(k), \psi_{\bar{\Omega}F_F)}(k)) \mid k \in U\}$$

Where $\mu_{\underline{\Omega}(F_F)}(k) = \wedge_{k_1 \in \Omega^*(k)} (\mu_{\mathcal{F}_{\mathcal{F}}}(k_1))$ and

$\psi_{\underline{\Omega}(F_F)}(k) = \vee_{k_1 \in \Omega^*(k)} (\psi_{\mathcal{F}_{\mathcal{F}}}(k))$

Which satisfies the condition $0 \leq (\mu_{\underline{\Omega}(F}{}_{F})(k))^3 + (\psi_{\underline{\Omega}(F}{}_{)}(k))^3 \leq 1$ and

$\mu_{\bar{(}\bar{\Omega}F}{}_{F})(k) = \vee_{k_1 \in \Omega^*(k)} (\mu_{\mathcal{F}_{\mathcal{F}}}(k_1))$ and

$\psi_{\bar{(}\Omega F_F)}(k) = \wedge_{k_1 \in \Omega^*(k)} (\psi_{\mathcal{F}_{\mathcal{F}}}(k))$

Which satisfies the condition $0 \leq (\mu_{\bar{\Omega}F}{}_{F})(k))^3 + \psi_{\bar{\Omega}F}{}_{F})(k))^3 \leq 1$

The pair $(\underline{\Omega}(F_F), \bar{\Omega}(F_F))$ is known as Soft rough fermatean fuzzy set with respect to (U, E, Ω) where $\underline{\Omega}(F_F) \neq \bar{\Omega}(F_F)$. The operators $\underline{\Omega}(F_F), \bar{\Omega}(F_F): FFS(E) \to FFS(U)$ are known as lower and upper soft rough fermatean fuzzy approximation operators with respect to (U, E, Ω).

Example 3.1

Suppose $U = \{k_1, k_2, k_3, k_4, k_5\}$ and $E = \{x_1, x_2, x_3, x_4\}$ be the initial set of parameters. A soft set (F, E) over U is defined as

$$F(x_1) = \{k_1, k_4\}, F(x_2) = \emptyset, F(x_3) = \{K_2, k_3\}, F(x_4) = \text{U}$$

Define a crisp soft relation Ω on $U \times E$,

$\Omega = \{(k_1, x_1), (k_2, x_4), (k_2, x_3), (k_3, x_2), (k_4, x_1), (k_4, x_3), (k_5, x_1), (k_1, x_3), (k_3, x_4)\}$

$$\Omega^*(k_1) = \{x_1, x_3\}$$
$$\Omega^*(k_2) = \{x_3, x_4\}$$
$$\Omega^*(k_3) = \{x_2, x_4\}$$
$$\Omega^*(k_4) = \{x_1, x_3\}$$
$$\Omega^*(k_5) = \{x_1\}$$

Define a fermatean fuzzy set on E as,

$$F_F = (x_1, 0.9, 0.5), (x_2, 0.9, 0.6), (x_3, 0.8, 0.7), (x_4, 0.8, 0.6)$$

Lower approximation space is

$$\underline{\Omega}(F_F) = \{(k_1, 0.8, 0.7), (k_2, 0.8, 0.7), (k_3, 0.8, 0.6), (k_4, 0.8, 0.7), (k_5, 0.9, 0.5)\}$$

Upper approximation space

$$\bar{\Omega}(F_F) = \{(k_1, 0.9, 0.5), (k_2, 0.8, 0.6), (k_3, 0.9, 0.6), (k_4, 0.9, 0.5), (k_5, 0.9, 0.5)\}$$

2. Fermatean fuzzy soft rough set (FFSRS)

In this section, we originate a new notion of FFSRS on the basis of Pythagorean fuzzy soft rough set (Hussain et al., 2020).

Definition 4.1

Let E be the set of parameters and U be the universal set. Then (F, E) is said to be Fermatean fuzzy soft set over U, if $F: E \to FFS(U)$ such that $\forall x \in E$,

$$F(x) = \{(k, \mu_{F(x)}(k), \psi_{F(x)}(k)) \,|k \in U\} \in FFS(U)$$

where $\mu_{F(x)}(k), \psi_{F(x)}(k) \in [0,1]$ represents membership and non-membership grade which satisfies $\mu_{F(x)}(k))^3 + \psi_{F(x)}(k))^3 \leq 1$

Definition 4.2

let E be the set of parameters and U be the universal set. Suppose Ω be the fuzzy soft relation on U. Then the triplet (U, E, Ω) is said to be fuzzy soft approximation space.

For any $F_F = \{(x, \mu_{\mathcal{F}_\mathcal{F}}(x), \psi_{\mathcal{F}_\mathcal{F}}(x)) \,|x \in E\} \in FFS(E)\}$ then the lower and upper approximations of F_F with respect to (U, E, Ω) are represented by $\underline{\Omega}(F_F) and \bar{\Omega}(F_F)$ and are defined as

$$\underline{\Omega}(F_F) = \{\, (k, \mu_{\underline{\Omega}(F_F)}(k), \psi_{\underline{\Omega}(F_F)}(k)) \mid k \in U\}$$

$$\bar{\mathbb{Q}}F_F) = \{ (k, \mu_{\bar{\mathbb{Q}}F_F)}(k), \psi_{\bar{\mathbb{Q}}F_F)}(k)) \mid k \in U\}$$

where $\mu_{\underline{\Omega}(F_F)}(k) = \wedge_{x\in E} \{ (1 - \mu_\Omega(k,x)) \vee \mu_{\mathcal{F}_\mathcal{F}}(x)\}$ and

$$\psi_{\underline{\Omega}(F_F)}(k) = \bigvee_{x\in \mathrm{E}} \{ \mu_\Omega(k,x) \wedge \psi_{\mathcal{F}_\mathcal{F}}(x)\}$$

also

$\mu_{\bar{\mathbb{Q}}F_F)}(k) = \vee_{x\in \mathrm{E}} \{ (\mu_\Omega(k,x)) \wedge \psi_{\mathcal{F}_\mathcal{F}}(x)\mu_{\mathcal{F}_\mathcal{F}}(x)\}$ and

$$\psi_{\bar{\mathbb{Q}}F_F)}(k) = \bigwedge_{x\in E} \{ (1 - \mu_\Omega(k,x)) \vee \psi_{\mathcal{F}_\mathcal{F}}(x)$$

Then the pair $(\underline{\Omega}(F_F), \bar{\mathbb{Q}}F_F))$ is known as fermatean fuzzy soft rough set (FFSRS) of F_F with respect to (u, E, Ω). where $\underline{\Omega}(F_F) \neq \bar{\mathbb{Q}}F_F)$. The operators $\underline{\Omega}(F_F), \bar{\mathbb{Q}}F_F): FFS(E) \to FFS(U)$ are known as lower and upper fermatean fuzzy soft rough approximation operators with respect to (U, E, Ω).

Here we will show that $\underline{\Omega}(F_F), \bar{\mathbb{Q}}F_F) \in FFS(U)$

$$\mu_{\underline{\Omega}(F_{\ }')}(k)^3 + \psi_{\underline{\Omega}(F_{\ }')}(k)^3$$

$$= \bigwedge_{x\in E} \{1 - \mu_\Omega(k,x)^3) \vee \mu_{\mathcal{F}_\mathcal{F}}(x)^3\} + \bigvee_{x\in \mathrm{E}} \{ \mu_\Omega(k,x)^3 \wedge \psi_{\mathcal{F}_\mathcal{F}}(x)^3\}$$

$$= 1 - \bigvee_{x\in \mathrm{E}} \{ \mu_\Omega(k,x)^3 \vee 1 - \mu_{\mathcal{F}_\mathcal{F}}(x)^3\} + \bigvee_{x\in \mathrm{E}} \{ \mu_\Omega(k,x)^3 \wedge \psi_{\mathcal{F}_\mathcal{F}}(x)^3\}$$

$$\leq 1 - \bigvee_{x\in \mathrm{E}} \{ \mu_\Omega(k,x)^3 \vee 1 - \mu_{\mathcal{F}_\mathcal{F}}(x)^3\} + \bigvee_{x\in \mathrm{E}} \{ \mu_\Omega(k,x)^3 \wedge 1 - \mu_{\mathcal{F}_\mathcal{F}}(x)^3\} = 1$$

Therefore $\underline{\Omega}(F_F) \in FFS(U)$. Similarly, we can show that $\bar{\mathbb{Q}}F_F) \in FFS(U)$

The operators $\underline{\Omega}(F_F), \bar{\mathbb{Q}}F_F): FFS(E) \to FFS(U)$ are called lower and upper approximation operators with respect to (U, E, Ω)

Example 4.1

Let $U = \{k_1, k_2, k_3, k_4, k_5\}$ and $E = \{x_1, x_2, x_3, x_4\}$ be the initial set of parameters. Consider a fuzzy soft set (F, E) over U, a fuzzy soft relation Ω from $U \times E$ is defined as

Ω	x_1	x_2	x_3	x_4
k_1	0.8	0.6	0.5	0.7
k_2	0.9	0.3	0.4	0.1
k_3	0.3	0.7	0.8	0.6
k_4	0.2	0.8	0.3	0.2
k_5	0.5	0.9	0.6	0.7

Define a fermetean fuzzy set

$$F_F = (x_1, 0.9, 0.5), (x_2, 0.6, 0.9), (x_3, 0.8, 0.7), (x_4, 0.8, 0.6)$$

Then $\underline{\Omega}(F_F), \bar{\Omega}(F_F)$ are

$$\underline{\Omega}(F_F) = (k_1, 0.6,0.6), (k_2, 0.7,0.5), (k_3, 0.6,0.7), (k_4, 0.6,0.8), (k_5, 0.6,0.8)$$

$$\bar{\Omega}(F_F) = (k_1, 0.6, 0.6), (k_2, 0.5, 0.7), (k_3, 0.7, 0.6), (k_4, 0.6, 0.7), (k_5, 0.6,0.6)\}$$

APPLICATION OF FERMATEAN FUZZY SOFT ROUGH SETS IN DECISION MAKING

The technique for the Decision making process is constructed on the approach of FFSRS . It is more effective to deal with DM problem with the evaluation of Fermatean fuzzy information based on SRFFS and FFSRS models than DM problems with the evaluation of SRPFS and PFSRS models.

Let (U, E, R) be a fuzzy soft approximation space, where U is the universe of the discourse, E is the parameter set, and R is a fuzzy soft relation on U×E. Then we can give an algorithm based on FF soft rough sets with five steps

- Step 1: construct a fuzzy soft relation R from U to E, or fuzzy soft set (F, E) over U
- Step 2: Construct an optimum normal decision object A on the basis of assumption, according to different needs of the decision maker.
- Step 3: we can compute the FF soft rough approximation operators $\underline{\Omega}(A) and\, \bar{\Omega}(A)$ of the optimum normal decision object A
- Step 4: By the ring sum operation, we can compute the choice set. we

should take the object $u_j \in U$ in universe U with the maximum choice value as the optimum decision for the given decision making problem.

- Step 5: Go back to the second step and change decision object so that the final decision is only one, when there exist too many "optimal choices" to be chosen

Example

Suppose that U= $\{u_1, u_2, u_3, u_4, u_5\}$ is the set of five houses under consideration of a decision maker to purchase. Let E be a parameter set, where E= $\{e_1, e_2, e_3, e_4, e_5\}$= {expensive; beautiful; size; location}. Mr. X wants to buy the house which qualifies with the parameters of E to the utmost extent from available houses in U. Assume that Mr. X describes the "attractiveness of the houses" by constructing a fuzzy soft set (F, E) which is a fuzzy soft relation from U to E. And it is presented by a table as in the following form:

R	e_1	e_2	e_3	e_4
u_1	0.7	0.1	0.5	0.3
u_2	0.2	0.5	0.8	0.7
u_3	0.3	0.3	0.1	0.6
u_4	0.5	0.5	0.2	0.4
u_5	0.5	0.4	0.1	0.8.

Now suppose that Mr. X gives the optimum normal decision object A which is a Fermatean Fuzzy subset defined as follows:

A= $(e_1, 0.9, 0.5), (e_2, 0.6, 0.9), (e_3, 0.8, 0.7), (e_4, 0.8, 0.6)$

$\underline{\Omega}(A) = \{(u_1, 0.6,0.6), (u_2, 0.7,0.5), (u_3, 0.6,0.7), (u_4, 0.6,0.8), (u_5, 0.6,0.8)\}$

$\overline{\Omega}(A) = \{(u_1, 0.6,0.6), (u_2, 0.5, 0.7), (u_3, 0.7,0.6), (u_4, 0.6,0.7), (u_5, 0.6,0.6)\}$

$\overline{\Omega}(A) \oplus \underline{\Omega}(A)$=

$\{(u_1, 0.84, 0.36), (u_2, 0.85, 0.35), (u_3, 0.98, 0.42), (u_4, 0.84, 0.56), (u_5, 0.84,0.48)\}$

Obviously optimum solution is u_3. Mr. X will buy the house u_3.

1. CONCLUSION

The theories of rough set, soft set, Intuitionistic fuzzy set, Pythagorean fuzzy set and Fermatean Fuzzy Set all are important mathematical tools for dealing with uncertainties. In this paper, we have presented two new concepts: SoftRough Fermatean Fuzzy Set and Fermatean Fuzzy Soft Rough Set. By combining crisp soft relation with soft rough approximation space, soft rough fermatean fuzzy approximation operators are defined. Also a new notion of Fermatean fuzzy soft rough set on the basis of Pythagorean fuzzy soft rough set is introduced. For that first we define a fermatean fuzzy soft set. Using a fuzzy soft relation, a fuzzy soft approximation space is defined and from that fermatean fuzzy soft rough approximation operators were defined.

These concepts can be very helpful in decision making problems. This method provides more freedom for the decision makers to the selection of membership and non-membership degrees as compared to existing literature and also it is more superior than the existing one

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INVITRO AND IN SILICO STUDIES OF CERTAIN CURCUMIN ANALOGUES' ANTIBACTERIAL EFFECT

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ABSTRACT

Curcumin analogues are widely used in numerous biological disciplines. They are widely employed in the pharmaceutical sector and offer good pharmacology application prospects in the present era. In the current study, two curcumin analogues—(1E,6E)-1,7-diphenylhepta-1,6-diene-3,5-dione (DPHDD) and (1E,6E)-1,7-bis(3,4-dimethoxyphenyl) hepta-1,6-diene-3,5-dione(BDMPHDD)—were tested in vitro against the bacterial strain *Staphylococcus aureus*.The testing demonstrated that the ligands may have antibacterial potential. The Lipinski rule of five was used to pre-filter the compounds' drug-like characteristics prior to computer analysis. Then, to determine the mechanism by which the compounds limit the growth of S. aureus, molecular docking research was carried out using the AutoDock 4.2 tool.Six distinct target proteins from S. aureus were chosen for this purpose (PDB ID: 1T2P, 3U2D, 2W9S, 1N67, 2ZCO, and 4H8E). The target protein *Dihydrofolate reductase* enzyme (PDB ID: 2W9S) and *Staphylococcus aureus sortase-A* (PDB ID: 1T2P) demonstrated a good binding affinity for the two analogues, (BDMPHDD) & (DPHDD) respectively. Due to the inactivation of these enzymes, the substances(1E,6E)-1,7-diphenylhepta-1,6-diene-3,5-dione (DPHDD) and (1E,6E)-1,7-bis(3,4- dimethoxyphenyl) hepta-1, 6-diene-3,5-dione (BDMPHDD) exhibit significant growth-inhibitory potential against *S. aureus*.

Key Words: Curcumin analogue, Antibacterial study, Molecular docking.

INTRODUCTION

Therapeutic research is crucial for lowering the incidence of human diseases and improving human quality of life. Pathogenic organisms are responsible for many diseases. One of these multi-drug-resistant bacteria is *S. aureus*. This bacterium is naturally present on the skin and in the nasopharynx of humans. Infections of the nose, skin, vagina, urethra and digestive system can be brought on by *S. aureus*[1,2]. Although there are many different antibiotics and chemotherapeutic drugs available to treat these bacteria, due to their high cost, only individuals with severely resistant strains should use them. The development of innovative and potent chemotherapy medications is therefore essential for the medical sector.

MATERIALS AND METHODS

1.1 . In silico molecular docking studies

ChemSketch software was used to determine the structure of the curcumin analogues in MOL format, and open babel software was used to transfer the structure to PDB format. Protein structures were retrieved from RCSB PDB in PDB format. Hydrogen atoms were added and the proteins' existing ligands and water molecules were removed using Pymol software before being saved in PDB format.

1.1.1 Lipinski rule of five: According to the Lipinski rule, an orally active medication will be tiny and somewhat lipophilic. According to this criterion, which illustrates molecular characteristics rather than pharmacological

action, a medicine has strong oral activity if it meets the five requirements.

1.1.2 Molecular docking: To determine the mechanism through which the curcumin analogues inhibit bacterial growth, docking tests were conducted. Docking studies were used to determine the binding affinities and interactions of these drugs with various target proteins in *S. aureus*. The PDB IDs for the chosen target molecules were 1T2P, 3U2D, 2W9S, 1N67, 2ZCO, and 4H8E. The protein—curcumin analogue adducts' binding energies were learned using molecular docking calculations using the Auto Dock 4.2 programme [3]. The 3D and 2D interaction graphs of the protein-ligand complexes were created using the software BIOVIA Discovery Studio.

1.2 . Preparation and Characterization of Curcumin Analogues

In an ethyl acetate medium with tributyl borate and n-butyl amine, aldehydes (benzaldehyde and 3,4- dimethoxy benzaldehyde) were coupled with an acetylacetone-boric oxide complex to create curcuminoid mimics. The products were refined using a 5:1 (v/v) chloroform: acetone mixture as the eluent in column chromatography over silica gel (60-120 mesh) and recrystallized twice from hot benzene in order to get pure crystalline content.IR, ^{13}C NMR, ^{1}H NMR, and mass spectrum methods are used to characterize the ligands.

1.3 . In vitro Antibacterial Studies

The Agar well diffusion method is frequently used to assess the test sample's antibacterial activity. Mueller-Hinton agar (15–20 mL) was put onto identical-sized glass petri plates and allowed to set. Using a sterile cotton swab, a standardised inoculum of the test organism was evenly distributed across the surface of the plates. A sterile cork borer was used to aseptically punch four 8 mm-diameter wells spaced 20 mm apart into each plate. The test sample (40 and 80 L) from the 10 mg/ml stock was added into wells T1 and T2. As a positive and negative control, gentamycin (40 l from a 4 mg/ml stock) and the solvent used for sample dilution, respectively, were added. The plates were incubated for 24 h at 36ºC ± 1ºC, under aerobic conditions. After incubation, the plates were observed and the zone of bacterial growth inhibition around the wells was measured in mm.

RESULT AND DISCUSSION

To assess for drug-like qualities, the compounds were first pre-filtered using Lipinski's rule of five. The properties of the two analogues, including their masses, hydrogen bond donors and acceptors, log P (the octanol-water partition coefficient), and molar refractivity were assessed using the rule and are shown in Table 1. According to this rule,an orally active drug is must have less than two violations[4]. Results showed that both the compounds have no violations and hence they obey the Lipinski rule, suggesting that these compounds have the potential to behave as orally active drugs.

It is now crucial to comprehend the process by which the chemicals prevent bacterial development. In order to determine which protein target in bacteria the ligands have the strongest binding affinity for, molecular docking studies were carried out. The greatest binding energy and the number of interactions between the ligand and the active site

residues were used to determine the stability of the protein-ligand complex .Hydrogen bond interactions such as conventional and non-conventional H-bonds, hydrophobic interactions such as pi-sigma, alkyl and pi-alkyl interactions, electrostatic interactions such as pi-anion interactions, van der Waals interaction, and unfavourable pi-donor interactions are commonly seen between protein and ligand. The binding affinity of the compound with the target protein is the result of all the interactions and binding energy existing between them. The highest binding energies (BE) and the number of interactions of the ligands with protein models under study were enlisted in Table 2.

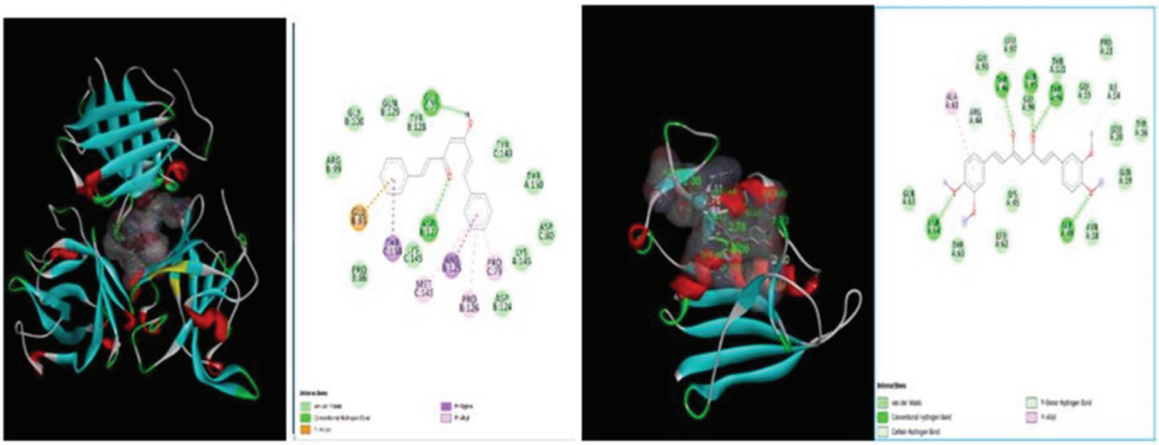
Table 1Lipinski Rule of Five

Lipinski rule of five			
Parameters	**Ligands**	**Conditions for Druglike property**	
	dphdd	**bdmphdd**	
Molecular weight g/mol	276.33	396.43	< 500
Hydrogen Bond Donor	1	1	< 5
Hydrogen Bond Acceptor	2	6	< 10
log P	3.96	3.91	< 5
Molar Refractivity	86.67	112.64	40–130

Table 2 Docking scores and No.of Interactions

Active Target	2W9S		1N67		1T2P		2ZCO		3U2D		4H8E	
Ligands	dphdd	bdmphdd	dphdd	bdmphdd	dphdd	bdmphdd	dphdd	bdmphdd	dphdd	bdmphdd	dphdd	bdmphdd
Active Site and Run	9	1	2	1	7	3	3	1	2	9	3	6
BE(kcal/mol)	-8.7	-9.4	-8.5	-8.96	-9.8	-7.48	-7.62	-6.73	-7.89	-7.3	-9.4	-8.4
Ligand efficiency	-0.4	-0.3	-0.4	-0.17	-0.5	-0.26	-0.36	-0.23	-0.38	-0.3	-0.45	-0.3
inhib constant (nM)	394	120	758.6	231.2	69.5	3.27	2.6	11.6	1.65	4.66	128.6	692
intermolar energy	-11	-12	-10.1	-7.94	-12	-10.5	-9.41	-9.71	-9.68	-10	-11.2	-11
vdw hb disolv energy	-10	-12	-10.1	-7.97	-12	-9.92	-9.39	-9.78	-9.73	-10	-11.1	-11
electrostatic energy	-0.1	-0.1	-0.07	0.02	-0	-0.54	-0.02	0.07	0.05	-0.1	-0.07	-0
total internal	-0.9	-1.2	-1.18	-1.78	-1.2	-1.85	-1.31	-1.94	-1.41	-1.9	-0.7	-1.7
torsional energy	1.79	2.98	1.79	2.98	1.79	2.98	1.79	2.98	1.79	2.98	1.79	2.98
unbound energy	-0.9	-1.2	-1.18	-1.78	-1.2	-1.85	-1.31	-1.94	-1.41	-1.9	-0.7	-1.7
cRMS	0	0	0	0	0	0	0	0	0	0	0	0
refRMS	40.8	39	81.12	86.97	24.4	39.1	78.49	57.6	25	24	26.29	23.7
rseed1	None	None	None	None	None	None	None	None	None	None	None	None
rseed2	None	None	None	None	None	None	None	None	None	None	None	None
Van der Waals	13	14	12	13	11	4	11	8	6	7	11	12
Hydrogen bond	1	5	2	2	2	2	0	1	2	2	2	3
Others	5	3	3	5	6	13	7	6	6	10	5	14
Total Interactions	19	22	17	20	19	19	18	15	14	19	18	29

The following Figures showing the Binding pockets and Protein Ligand Interactions.



The curcumin analogues were synthesized in the wet lab by Pabon's Method and the characterization by various spectral analyses was conducted. Spectral Data are shown in Tables 3,4,5 and 6.

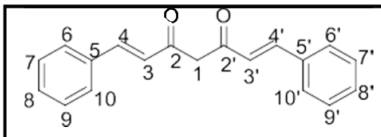
Table 3 IR Data

DPHDD	BDMPHDD	Probable IR Assaignments
3040	2929	ν Enolic
1622	1620	ν (C=O)Chelated
1581	1585	ν (C=C)Phenyl
1512	1507	ν (C-C)Alkenyl
1456	1466	ν as(C-C-C)Chelate ring
1426	1423	ν s(C-C-C)Chelate ring
1145	1121	ν β(C-H)Chelate ring
968	958	ν (CH=CH)trans

Table 4 ^{1}H NMR and Mass Spectral Data

Ligands	Chemical shift(δ) in ppm					Mass spectral data (m/z)
	Enolic	Methine	Alkenyl	Phenyl	Substituent	
DPHDD	10.014	6.78	6.98-7.79	7.31-7.60	---	276,199,173,145,131,103,90,77
BDMPHDD	9.84	6.75	6.81-7.61	7.06-7.14	3.85 (methoxy)	396,259,233,205,191,137,163

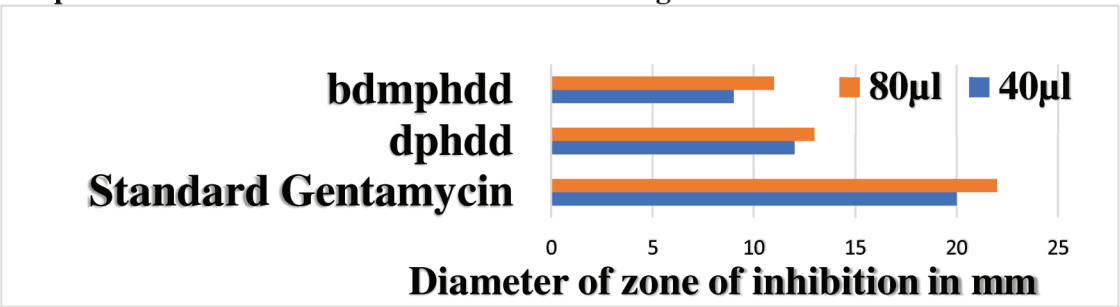
Table 5 ^{13}C NMR Data of DPHDD



C1	C2,C2'	C3,C	C4,C4'	C5,C5'
98.63	200.99	130.26	130.26	133.76
C6,C6'	**C7,C7'**	**C8,C8'**	**C9,C9'**	**C10,C10'**
128.57	128.57	128.57	128.57	128.57

The ligands BDMPHDD & DPHDD have the potential to function as effective antibacterial agents, according to an in vitro antibacterial investigation (Graph 1). Despite having less action than the common antibiotic gentamycin, both BDMPHDD and DPHDD have noticeable growth-inhibitory potential. At an 80 l well-1 concentration, gentamycin's zone of inhibition on S. aureus measured 22 mm in diameter, whereas the analogues BDMPHDD & DPHDD measured 11 mm & 13 mm, respectively. It was discovered that the zone of inhibition grew larger as the chemical concentration did. Thus, they can be consideredgoodantibacterialagentsfor*S.aureus.*

Graph 1 Antibacterial Effects of Curcumin Analogues



CONCLUSION

The two curcumin analogues (1E,6E)-1,7-diphenylhepta-1,6-diene-3,5-dione (DPHDD) and (1E,6E)-1,7-bis(3,4-dimethoxyphenyl) hepta-1,6-diene-3,5-dione (BDMPHDD) exhibit significant growth-inhibitory potential on comparing with the inhibitory power of the standard antibiotic gentamycin against the pathogenic bacteria *S.aureus*. Maximum zone of inhibition of about 13mm and 11mm were shown by DPHDD and BDMPHDD, respectively, at a concentration of 80ìlwell[1]. Both obeyed Lipinski's rule of five and possess drug- like properties. Among the target proteins selected for study, the target protein *Dihydrofolate reductase* enzyme (PDB ID: 2W9S) and *Staphylococcus aureus sortase-A* (PDB ID: 1T2P) demonstrated a good binding affinity for the two analogues, (BDMPHDD) & (DPHDD) respectively which clearly establish that the appreciable growth-inhibitory power of these curcumin analogues against the pathogenic bacteria *S. aureus* is mainly due to deactivation of the enzymes, *Dihydrofolate reductase* and *Staphylococcus aureus sortase-A*.

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EVALUATION OF ANTIGENOTOXIC POTENTIAL OF TURMERIC EXTRACT AGAINST SODIUM POTASSIUM TARTRATE, A FOOD ADDITIVE

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ABSTRACT

Turmeric, the 'Golden spice' is the rhizome of Curcuma longa, which is a member of the family Zingiberaceae. Curcumin, the principal curcuminoid found in turmeric is the most active ingredient of the turmeric that gives its characteristic properties. The present study analyses the chromosomal aberrations that can be induced by Sodium potassium tartrate, a meat preservative in Onion root meristem cells and the efficiency of natural turmeric powder in reducing the cytotoxic effect of Sodium potassium tartrate. The concentrations of Na K tartrate used were 0.01%, 0.1%, 1% and 10% and observations were made on germination percentage, mitotic index, mitotic aberrations and frequency of mitotic aberrations. The efficacy of turmeric was assessed by the pre-exposure, co-exposure and post exposure treatments. The Co - exposure was found to be better than pre- exposure and post exposure as the former showed more mitotic index and reduced frequency of aberrations than the other two. Pre exposure showed better results than post exposure because in former more mitotic index and reduced frequency of aberrations were observed than latter.

Key words: Turmeric, antigenotoxic potential, Na-K tartrate, mitotic aberrations, Onion root cells

INTRODUCTION

Food additives are substances intentionally added to foodstuffs to perform specific functions, such as to improve shelf life, to enhance colour, flavour or consistency. The use of this additives is a well-accepted practice but not without controversy. Many additives used in modern food industry, have been in use for centuries in the preparation of food ingredients such as salt, sugar and vinegar which have served as preserving agents for thousands of years. The safety of all food additives that are currently authorized has been assessed by the Scientific Committee on Food (SCF) and the European Food Safety Authority (EFSA).

A preservative is a substance or a chemical that is added to products such as food, beverages, pharmaceutical drugs, paints, biological samples, cosmetics, wood and many other products to prevent decomposition by microbial growth or by undesirable chemical changes. In general, preservation is implemented in two modes, chemical and physical. Chemical preservation entails adding chemical compounds to the product. Physical preservation entails processes such as refrigeration or drying.

Since pre historic times, chemicals have been added to foods to perform special functions. Although basic food contains no additives, in processed food many alternatives are used. Technological advances in food processing have increased the variety and use of these additives. Today more than 2500 different additives are intentionally added to foods to produce desired effect. The use of this

additives is a well-accepted practice but not without controversy.

METHODOLOGY

a. Range Finding Test

To find out the suitable concentrations of the chemical (Sdium potassium tartrate) to be used in the experiment, range finding test was conducted using the concentrations 0.01%,0.1%,1% and 10%. From the results obtained, concentrations of sodium potassium tartrate that can be used in the assay were fixed as 0.01%, 0.1%, 1% and 10%.

b. Preparation of turmeric powder

For the preparation of turmeric powder, fresh rhizomes of *Curcuma longa* were collected. These were washed thoroughly, chopped into pieces and were dried in open sunlight. Dried rhizome was ground to make fine powder of turmeric.

c. Preparation of turmeric extract

20g of turmeric powder was weighed out accurately using an electronic weighing balance and was dissolved in 200ml distilled water. The mixture was kept in shaker for 24 hours. It was then filtered using filter paper to obtain10% stock solution. From the 10% stock solution, 5 mg/ ml extract was made by pipetting out 5 ml extract into a measuring cylinder and making the final volume to 100ml.

d. Test for antigenotoxicity

To study the antigenotoxic effect of turmeric, three sets of experiments were conducted as follows:

Pre - exposure

20ml of 5mg/ml *Curcuma longa* rhizome turmeric extract was added to first set of onion containing petriplates and kept for 24 hours. Then the bulbs were washed with distilled water and exposed to equal amount of different concentrations of test solution for another 24 hours. The control was supplied with only distilled water.

Co - exposure

20 ml of both chemical and *Curcuma longa* rhizome extract were simultaneously added to the second set of petriplates. Then after 48 hours, the root tips were fixed after washing with distilled water.

Post - exposure

The onions were first treated with 20 ml of respective concentrations of test solution for 24 hours. After the pre-treatment, the bulbs were washed and exposed to the same amount of extract. The petriplates were kept at room temperature for 48 hrs. for the germination of onion bulbs. After 48 hrs., the germinated bulbs were washed in distilled water for the removal of test solutions. The root tips were cut with razor blade and fixed in Carnoy's fluid. The microscopic preparations were developed by chromosome squash technique.

Photomicrographs of cells under mitosis and different mitotic abnormalities were taken using computer connected with Labomed Photo micrographic unit.

e. Analysis of the parameters.

Germination percentage (GP) =

$$\frac{Number\ of\ bulbs\ germinated}{Total\ number\ of\ bulbs}\ x\ 100$$

Mitotic index (MI) =

$$\frac{Number\ of\ dividing\ cells}{Total\ number\ of\ cells}\ x\ 100$$

Frequency of Mitotic aberrations =

$$\frac{Number\ of\ cells\ s\square owing\ aberrations}{Total\ number\ of\ dividing\ cells}\ x\ 100$$

g. Statistical Analysis

Results obtained were analyzed statistically to find out mean and standard deviation. One way ANOVA was performed for assessing the significance of the results.

RESULTS AND DISCUSSION

According to Grant (1982), Allium test has been used for the determination of genotoxic effect of various compounds and it is considered as the standard procedure for quick testing and detection of toxicity of food additives. In the current study, when onion bulbs are treated with sodium potassium tartrate for 48 hrs., higher germination percentage (100%), maximum number of roots /bulbs, maximum mitotic index (95%) and absence of mitotic aberrations were observed in control. Gradual decrease of germination percentage, no. of roots/bulb, mitotic index and increase in the appearance of mitotic aberrations were noted with increase of concentration of the chemical. Lower germination percentage, reduced no. of roots / bulb, minimum mitotic index, maximum mitotic aberrations and maximum frequency of aberrations were noted in higher concentrations of Na – K tartrate (table 1). Similar findings were observed in *Vinca faba* root cells (Pandey and Santhosh, 2007) and also in *Allium cepa* root cells treated with food additives other than sodium potassium tartrate (Faizah and Wahab, 2014; Palani et al., 2007; Sifa, 2005).

Different types of abnormalities revealed after treatment with Na - K tartrate in the present study were pulverized chromosome at metaphase, chained metaphase, chromosome clumping, sticky chromosome, dislocation of chromosome, diagonal metaphase, nuclear lesions, chromosome breakage, diagonal telophase, chromosome clumping at metaphase and strap shaped nucleus.

In recovery test, three types of exposures were given to onion bulbs *Curcuma longa* rhizome extract: Pre- exposure, Co-exposure and Post exposure. On treatment with *Curcuma longa* rhizome extract, an increase in mitotic index was noted compared to the chemical alone treated onion bulbs. Also, the frequency of mitotic aberrations was decreased. The type of aberrations was also reduced and it shows the antigenotoxic effect of *Curcuma longa* against chemicals. The Co -exposure was found to be better than pre-exposure and post exposure because the former showed more mitotic index and reduced frequency of aberrations than the other two. Then pre- exposure is found to be better than post exposure because in pre - exposure more MI and reduced frequency of aberrations were observed compared to post - exposure (table1).

The results indicate that the consumption of food containing these additives along with the turmeric in any form is better than the consumption of food before or after the intake of this herbal product. The positive results with regard to the toxicity of Na - K tartrate in the *Allium* test should be considered as a warning and also an indication that the tested chemical may be a risk to human health and to our environment.

Table 1. Antigenotoxic potential of turmeric extract against Sodium potassium tartrate

Concentration	GP			Roots/bulb			MI			Frequency of aberrations		
	PrE	CE	PoE	PrE	CE	PoE	PrE	CE	PoE	PrE	CE	PoE
DIST.WATER	80	80	80	9	5	8	0.85	0.85	0.79	0	0	0
0.01	60	60	60	8	6	7	0.74	0.80	0.61	9.8	8.6	11.08
0.1	30	40	40	4	3	4	0.62	0.79	0.60	29.1	11.58	22.9
1	20	40	20	2	3	3	0.51	0.65	0.53	30.05	23.1	30.5
10	10	-	-	2	-	-	0.59	-	-	33.1	-	-

PrE-pre exposure, CE-Coexposure, PoE-Post Exposure

CONCLUSION

The present study revealed that sodium potassium tartrate, which is used frequently in food industry as preservative and flavouring agent have genotoxic effects. Further studies in animal models are needed to confirm harmful effect of sodium potassium tartrate if used as

food additive.

The study also confirmed the antimutagenic and

antigenotoxic property of turmeric rhizome extract which was responsible for the decrease in sodium potassium tartrate induced chromosomal aberrations. Co - exposure to turmeric was found to be more effective in overcoming the toxic effect of Na-K tartrate than pre- exposure and post- exposure. Further studies in this context are needed to understand the different mechanisms by which the rhizome extracts of *Curcuma longa* perform the protective role against harmful food additives.

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ECOFRIENDLY SYNTHESIS OF SILVER NANOPARTICLES FROM AQUEOUS LEAF EXTRACT OF PIPER NIGRUM L. AND EVALUATION OF ITS ANTIMICROBIAL ACTIVITY AGAINST INFECTIOUS PATHOGENS

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ABSTRACT

Piper nigrum commonly known as black pepper belonging to the family Piperaceae, is cultivated widely for its fruit which is usually dried and used as a spice. The current work analyzes the potential of the aqueous leaf extract of Piper nigrum to produce silver nanoparticle from AgNO3 solution and to assess its antibacterial activity. Formation of Ag nanoparticles was indicated by the change in the color of test solution from green brown to brown color. Formation of Ag nanoparticles was confirmed by UV visible spectral analysis, XRD and SEM studies. Ag particles obtained were found to be highly active against *Staphylococcus aureus* and *E. Coli* followed by *Pseudomonas aeruginosa* and *Bacillus subtilis.*

Key Words: Silver nanoparticle, aqueous extract, *Piper nigrum*, antibacterial activity

INTRODUCTION

Nanotechnology can be defined as the manipulation of matter through certain chemical and physical processes to create materials with specific properties which can be used in particular applications. A nanoparticle can be defined as a microscopic particle that has at least one dimension less than 100 nanometers in size with a surrounding interfacial layer. The interfacial layer is an integral part of nanoscale matter fundamentally affecting all of its properties. Different protocols have been designed for the production of metallic nanoparticles.

Piper nigrum commonly known as black pepper is a flowering vein belonging to the family Piperaceae, cultivated for its fruit known as pepper corn, which is usually dried and used as a spice. Black pepper is native either to Southeast Asia or South Asia. Pepper contains phytochemicals including amides, piperidines, Pyrolidines and trace amounts of safrole, which may be carcinogenic in laboratory rodents.

METHODOLOGY

Piper nigrum L. was collected from local areas of Thrissur. The plant material was dried in shade at ambient temperature and made it to powder by electric blender. The powdered material was stored in air tight containers for further use.

Preparation of plant extract

5g of fine powder was weighed and boiled with 100mL of deionized water at 80°c for 15 minutes using water bath. The plant extract was filtered and collected separately.

Synthesis of Silver Nanoparticles from plant extract

To 10ml of aqueous leaf extract of Piper nigrum L. 90mL of 1mM silver nitrate solution was added and observed the color change.

Characterization of Silver Nanoparticles

The synthesis of nanoparticles was confirmed and monitored with the help of the various

analytical methods like UV-Visible spectra, SEM, XRD and EDAX analysis

Phytochemical analysis of *Piper nigrum* leaves

Phytochemical screening was carried out in the deionized water extracts of *Piper nigrum* L. Primary metabolites analyzed were carbohydrates (Molisch's test), aldehyde (Fehling's test), sugar (Benedict test), ketose (Seliwanoff's test), starch, amino acids (ninhydrin test), fats (filter paper test).

Qualitative tests were conducted for various secondary metabolites like quinine (H_2SO_4 test), cardiac glycoside, steroids (Lieberman buchard test), alkaloids (Wagner's test), Terpenoides (saliskowski's test), phenol (folin's test), saponins (foam test), Tannins (iron salt test), coumarins, flavonoids, acid and resin. All the tests were carried out by using standard procedures (Harborne,1973; Sofowora,1982).

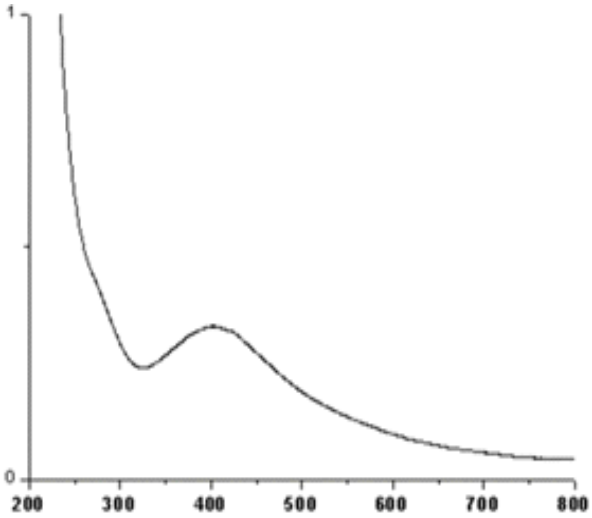
Antibacterial activity

Two human pathogenic gram negative (*Pseudomonas aeruginosa*, *E. Coli*) and two gram positive (*Staphylococcus aureus*, *Bacillus subtilis*) bacterial strains were used for antimicrobial study of Silver Nanoparticles by well diffusion method.

RESULTS AND DISCUSSION

Plant extract contains several phytochemicals that react with silver nitrate and converts it into silver nanoparticles ie. silver ions which were primarily identified by the colour change from greenish brown to brown in the reaction mixture immediately on addition. Synthesis of Ag nanoparticles was confirmed by the UV visible spectrophotometric analysis that showed the absorption maxima at 400 nm characteristic peak of Ag nanoparticles (Fig.1).

Fig.1. UV-VIS Spectrophotograph of AgNP



XRD analysis was performed to verify the presence of Ag particles at its domain planes. The result showed typical XRD pattern of Ag nanoparticle. The observed peaks were compared with the standard powder diffraction card (JCPDS file No. 87-0720) and the results were in agreement with the standard patterns of XRDs of AgNPs (fig.2). Energy dispersive X-Ray Analysis (EDAX) spectrum of the synthesized nanoparticles, suggests the presence of silver as the ingredient element. A typically strong signal peak at 3 keV in dispersive spectrum confirms the presence of Ag (fig.3). The SEM micrograph revealed that the synthesized silver nanoparticles were aggregated as irregular spherical shapes and ranges from 100-200 NM with inter particle distance (plate 1)

Fig.2. XRD of AgNPs

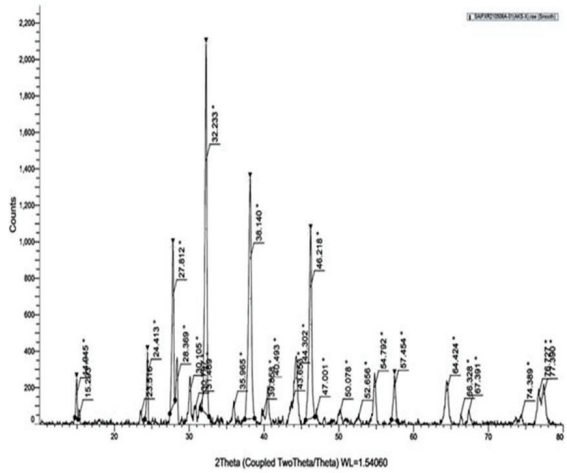


Fig.3. SEM –EDAX of AgNPs

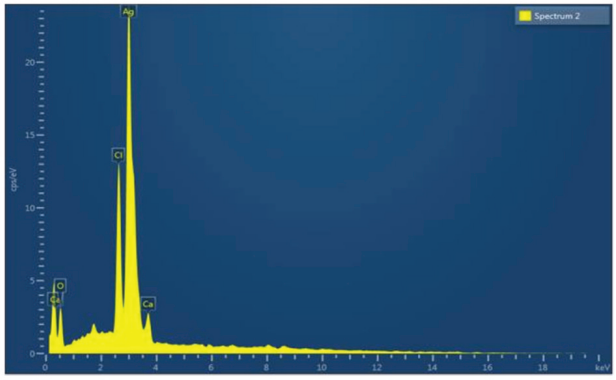
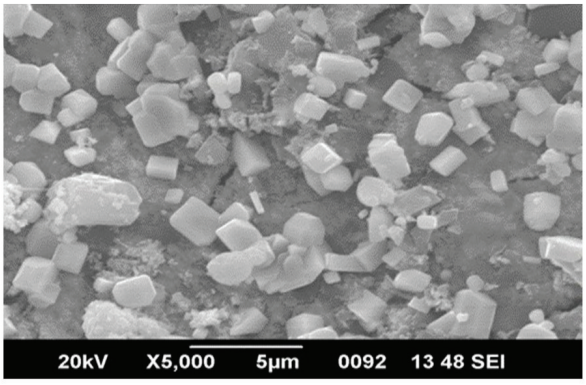


Plate 1. SEM analysis 500 X



Analysis of antibacterial activity revealed that the AgNPs were highly active against *staphylococcus aureus* and *E. Coli* followed by *Pseudomonas aeruginosa* and

then *Bacillus subtilis*. The results are depicted in table 1. Similar antibacterial activity of silver nano-particles was reported against *E.coli* and *Pseudomonas aeruginosa* (Jain et al., 2009); *Bacillus cereus* and *Pseudomonas aeruginosa* (Elumalai et al., 2010) *; Staphylococcus aureus*, *E.coli*, *Salmonella typhi* and *Candida albicans* (Dar et al., 2013).

CONCLUSION

The current reveals the potential of Piper nigrum leaves in the production of Ag nanoparticles from AgNO3 solution. Various techniques adopted for the analysis of nanoparticles confirmed the synthesis of Ag nanoparticles. Nanoparticles thus produced were found to be effective against various human pathogenic bacteria. The mechanism of synthesis of silver nanoparticles by plants can be used in the drug production for diseases which are caused by multidrug resistant bacteria.

Table 1. Antibacterial activity against various strains of bacteria

Organism	Zone of Inhibition in AgNPs (in mm)	Zone of Inhibition in Amoxycillin(in mm)
Staphylococcus aureus	**5**	**15**
Bacillus subtilis	**3**	**0**
Pseudomonas aeruginosa	**4**	**8**
E. coli	**5**	**10**

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ANATASE TO RUTILE PHASE TRANSFORMATION OF TiO2 NANOPARTICLES

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ABSTRACT

The anatase to rutile phase transformation of Titanium dioxide nanoparticles upon calcination is reported here. TiO2 nanoparticles are synthesized by sol gel method using titanium (IV)-n - butoxide (Ti(OC4H9)4 or Ti(OBu)4), isopropyl alcohol ((CH3)2CHOH) and conc. HNO3. The thermal stability and the decomposition of synthesized materials are studied using thermogravimetric (TG) analysis. The TGA studies show no weight loss for the sample after 400^{O}C. Hence the as prepared samples are calcined at 400 and 800^{O}C for three hours The structural characterization of the nanoparticles is done using X-ray diffraction (XRD) technique. The XRD patterns indicate that the structure of TiO2 is anatase at a calcination temperature of 400^{O}C and rutile at 800^{O}C. The X-ray diffraction studies show an increase in the intensity of diffraction peaks, decrease in FWHM and increase in crystallite size. The crystallite size values obtained are 11.3 and 58 nm for the anatase and rutile samples respectively. The optical absorption of these nanoparticles are investigated

using UV-Visible and photoluminescence (PL) spectroscopic methods. The optical absorption spectra of TiO2 sample exhibited strong absorption in the UV region. The band gap energy values obtained are 3.43 and 3.00 eV for the anatase and rutile samples respectively, in close agreement with the values obtained in other studies. The samples exhibit a strong and wide PL signal from 400 to 500 nm and a shoulder peak at 377 nm with an excited wavelength of 300 nm. Both the samples exhibit similar type of PL signal with no significant change in the curve shape. The emission intensity of anatase is higher than that of rutile sample. This study reports the successful transformation from anatase to rutile phase of TiO2 nano particles synthesized by sol gel method.

Keywords: TiO2 nanoparticles, anatase & rutile phase, sol-gel technique, phase transformation.

INTRODUCTION

With the advent of nanotechnology, the use of NPs in electronics, antimicrobial materials, cosmetics, sunscreens, and medication delivery systems has increased dramatically. Titanium dioxide nanoparticles, also known as ultrafine titanium dioxide or nanocrystalline titanium dioxide. Microcrystalline titanium dioxide or titanium dioxide are titanium dioxide particles with a diameter less than 100 nm. The metastable anatase phase of titanium dioxide produces nanoscale particles due to its lower surface energy than the equilibrium rutile phase. Surfaces of ultrafine titanium dioxide with anatase structures are useful as an addition in building materials such as anti-fogging coatings and self-cleaning windows due to their photocatalytic sterilising capabilities.

TiO2 is a significant compound due to its exceptional catalytic and semiconducting properties. It's also chemically stable, non-toxic,

and biocompatible. Nano TiO_2 is a powerful oxidising agent with a large surface area and, as a result, high photocatalytic activity. The refractive index of titanium dioxide (TiO_2) nanoparticles is 2.4. It is used in a variety of applications such as pharmaceuticals, coatings, inks, plastics, food, cosmetics, and textiles.

Anatase, Rutile, and Brookite are the three crystalline phases of titanium dioxide. Rutile and anatase are two of the three common TiO_2 polymorphs (crystal forms) used to make TiO_2 nanoparticles. TiO_2 nanoparticles, as opposed to large TiO_2 particles, are transparent rather than white. TiO_2 has unique electrical and diffusion path properties. TiO_2 nanoparticles are typically broad band gap semiconductors with Eg-values ranging from 3.0 to 3.2 eV and high UV absorbance.

Sol-gel, flame hydrolysis, co-precipitation, impregnation, and chemical vapour deposition processes are used to create TiO_2 nanoparticles. Researchers are particularly interested in the biosynthesis of titanium dioxide nanoparticles because it is a low-cost, environmentally friendly, and repeatable method.The sol-gel process is a wet-chemical method for producing high-quality metal-oxide-based nanomaterials. It is used in the production of TiO_2 nanoparticles. X-ray diffraction, UV-Vis spectroscopy, photoluminescence, and thermogravimetric analysis are all methods of characterization. When heated, anatase to rutile phase transformation can be seen. We successfully produced and transformed TiO_2 nanoparticles from anatase to rutile phase in this study. Its properties should also be studied using various

MATERIALS AND METHODS

Materials

All the chemicals used for the synthesis of titanium dioxide are of analytic reagent grade. The specific reagents used for the synthesis of titanium dioxide include titanium (IV)-n - butoxide ($Ti(OC_4H_9)_4$ or $Ti(OBu)_4$), 97%, Sigma-Aldrich), isopropyl alcohol ($(CH_3)_2CHOH$), 99%, Merck) and conc. HNO_3 (99.9%, Merck). Distilled water is used throughout the synthesis.

Synthesis of TiO2 NPs

The precursor solution is a combination of titanium (IV)-n-butoxide ($Ti(OBu)_4$) and isopropyl alcohol with a ratio of 1:2. This solution was then dropped into a distilled water solution while being stirred. A sol was generated after 3 hours of hydrolysis at room temperature and stirring. Finally, the produced sol was dried for 20 hours at 60! to get TiO_2 powder. The powder samples were then calcined for 3 hours in a furnace at 400! and 800!.

RESULT AND DISCUSSION

Figure 1 shows the thermogravimetric analysis of TiO2 NPs. The TG curve indicates that the weight loss of the as prepared sample occurred from 500 to 400 ! . This may be related to the decomposition of the residual titanium butoxide and organic compounds. This suggests that the synthesized sample decomposed completely by 400! to become titanium dioxide

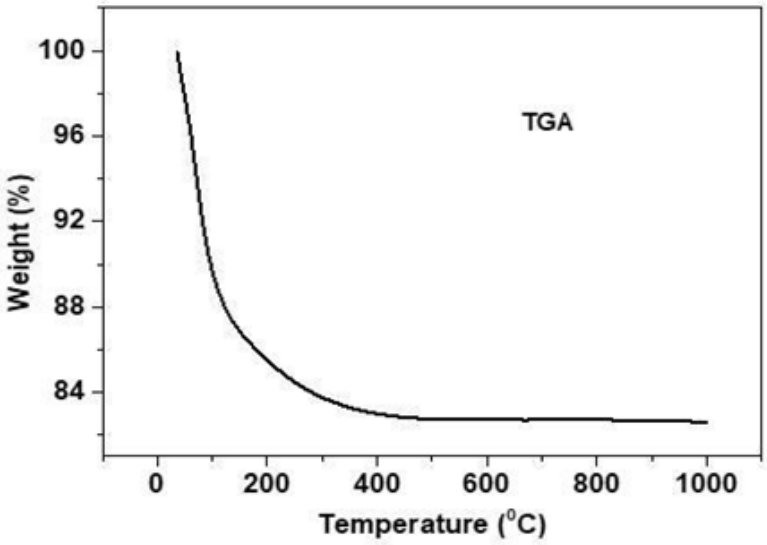

Fig: 1 TGA curve of TiO2

The XRD patterns show that TiO2 has an anatase structure at 400°C and a rutile structure at 800°C. The anatase ph ase found at 2è values of 25.357, 37.888, 48.024, 54.9, and 62.768 matches the convention al XRD pattern (JCPDS files No. 21-1272). The rutile phase of TiO2 is represented by the peaks at 2è values of 27.468, 36.095, 41.258, 44.076, 56.659, and 69.036 and is consistent with the conventional XRD pattern (JCPDS files No. 21-1276). When the calcination tempe rature is raised from 400°C to 800°C, a phase change from anatase to rutile occurs.

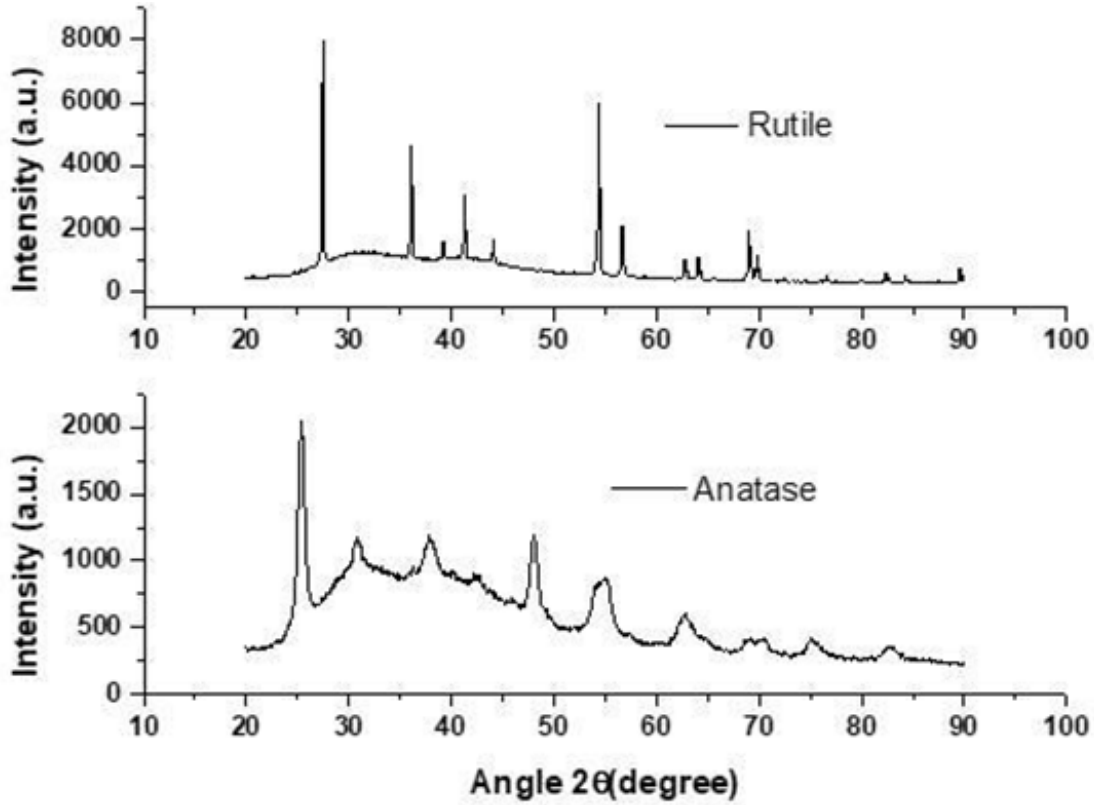

Fig: 2 XRD pattern of anatase and rutile TiO2 NPs

From this figure, it is observed that diffraction peaks become intense and their FWHM decreases on heating the sample from 400oC to 800oC, indicating an increase in crystallite size. The crystallite sizes of the samples are calculated from the line broadening of the diffraction peaks using Scherrer formula,

D=kë/âcosè

Where D represents the average crystallite size.k = 0.89 (Scherrer constant), ë = 1.5406 Å (wavelength of the X-ray Cu Ká radiation), è the diffraction angle of the peak and â represents the full-width at half-maximum (FWHM) of the peaks. The values obtained were 11.3 and 58 nm for the anatase and rutile samples respectively.

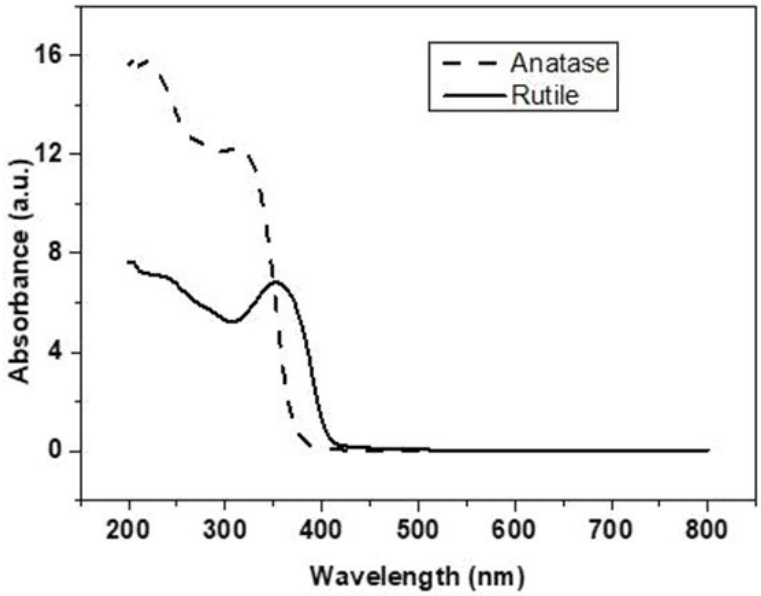

Fig: 3 UV-Vis absorption spectra of anatase and rutile TiO2 nanoparticles

Both samples have high UV absorption followed by an absorption hump between 300 and 400 nm. The electron transfer from the valence band to the conduction band is represented by UV absorption (band–band transition). The existence of Ti3+ vacancies created during annealing may explain the clearer hump in the rutile sample. During the phase change from anatase to rutile, a red shift occurs.

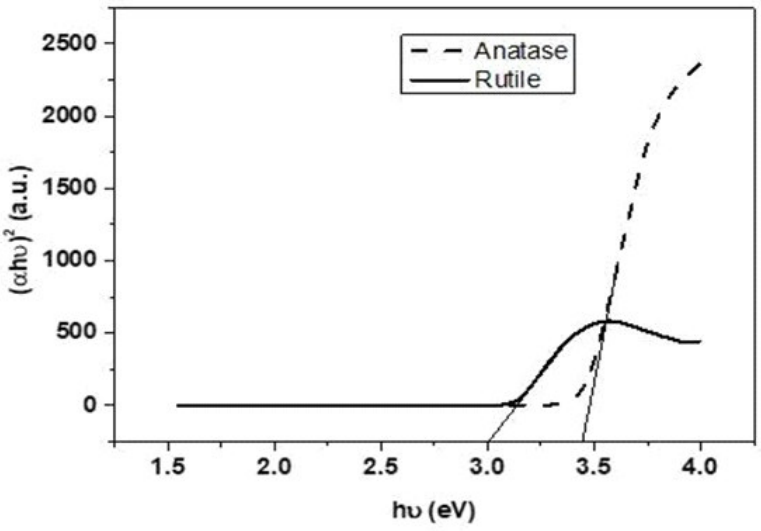

Fig: 4 Tauc Plot of TiO2 nanoparticles

Direct bandgap (Ed) of samples is determined by fitting absorption data to direct transition equation,

$$áhõ = Ed(hõ - Eg)^{½}$$

where á is optical absorption coefficient, hõ photon energy and a constant. Band gap of the samples have been measured by plotting as a function of photon energy hí and extrapolating linear portion of the curve to absorption equal to zero. The anatase and rutile samples had band gap energies of 3.43 and 3.00 eV, respectively. In general, rutile has a lower bandgap (about 3.05eV) than anatase phase and is the most thermostable form of TiO2. Figure 5 shows a strong and wide PL signal from 400 to 500 nm, as well as a shoulder peak at 377 nm and an excited wavelength of 300 nm. The shoulder peak is caused by direct recombination of electrons in the conduction band with holes in the valence band. The surface trap states are responsible for the emission peak at 470 nm. Both examples show a similar sort of PL signal with no discernible difference in curve form. The intensity of anatase emission is greater than that of rutile sample. The oxygen vacancy concentration increases as particle size decreases, and hence absorbance across the UV and visible range increases. Higher temperature annealing reduces the intensity of emission by decreasing defect centres of rutile phase

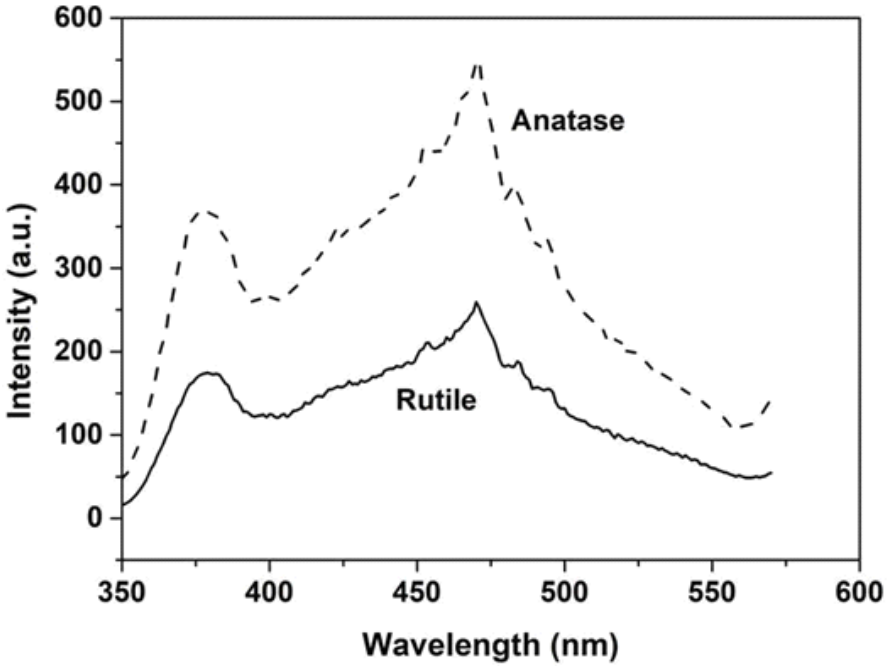

Fig:5 PL spectra of TiO2 nanoparticles

CONCLUSION

The sol-gel technique was used to successfully synthesise TiO2 NPs. The TGA experiments reveal that the sample loses no weight after being heated to 400^{O}C. As a result, the as-prepared samples are heated for three hours at 400 and 800^{O}C. X-ray diffraction investigations demonstrate a rise in the intensity of diffraction peaks, a decrease in FWHM, and an increase in crystallite size. The anatase and rutile samples had crystallite sizes of 11.3 and 58 nm, respectively. The optical absorption spectra of TiO2 sample showed high absorption in the UV range. A hump is visible between 300 and 400 nm, which is more visible in the rutile sample.The band gap energy values obtained for the anatase and rutile samples are 3.43 and

3.00 eV, respectively, which are in close agreement with the values obtained in other samples. The samples exhibit a strong and wide PL signal from 400 to 500 nm and a shoulder peak at 377 nm with an excited wavelength of 300 nm. Both examples show a similar sort of PL signal with no discernible difference in curve form. The intensity of anatase emission is greater than that of rutile sample.

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