



MKR GOVT. DEGREE COLLEGE

(Accredited with B++ Grade by NAAC, ISO 9001-2015)

Affiliated to Mahatma Gandhi University
DEVARAKONDA, NALGONDA,
TELANGANA



A REPORT

ON

BEST PRACTICES”



ORGANIZED

BY

DEPARTMENT OF CHEMISTRY

2020-2023



MKR GOVERNMENT DEGREE COLLEGE

(Accredited by NAAC with B++ Grade & ISO 9001 : 2015)

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Department of Chemistry

To enhance research aptitude in students, Department of Chemistry adopted and implemented the following best practice

S.No	Title of the Best Practice	Academic Year	Supervised by	Participating students
1	Student project on “Hydrogeochemical Characterization and Assessment of Ground water Quality Suitability for Drinking and Irrigation in Devarakonda area, Nalgonda district, Telangana state, India”	2021-2022	Dr M Alivelu	P Roja, M Praveen, M Kotesch, K Shirisha
2	Student project on “In-Silico ADME, Bioactivity and Toxicity prediction of some selected Antiviral drugs”	2021-2022	Dr M Alivelu	R Saritha, V Sandeep kumar, G Venkatesh, V Swami
3	Field project on “Detection of Food Adulterants”	2020-2021	Dr M Alivelu	1.A Jithendar, 2.A Ajay Kumar, 3.A Premalatha, 4.A Shiva, 5.A Anjali, 6.B Suresh

**Hydrogeochemical Characterization and Assessment of Groundwater Quality
Suitability for Drinking and Irrigation in Devarakonda area, Nalgonda
district, Telangana state, India.**



By

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**THE PROJECT REPORT SUBMITTED TO MAHATMA GANDHI UNIVERSITY IN
PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE DEGREE OF
UNDER GRADUATION IN CHEMISTRY**

JUNE-2022



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CERTIFICATE

This is to certify that the following mentioned students of Munagala Kondal Rao Govt. Degree College Devarakonda Nalgonda (Dt) have done the group project in chemistry with title: 'Hydrogeochemical Characterization and Assessment of Groundwater Quality Suitability for Drinking and Irrigation in Devarakonda area, Nalgonda district, Telangana state, India' under the supervision of Dr. M. Alivelu, Assistant professor of Chemistry of this college and submitted the same to the Department of Chemistry.

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Signature of the Principal

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DECLARATION

We the students of Munagala Kondal Rao Govt. Degree College are hereby declare that we have done this original research project our selves under the guidance of Dr. M. Alivelu, Asst. Professor of Chemistry, MKR, Govt. Degree College, Devarakonda. We declare that the work incorporated is original and same has not been submitted elsewhere for any degree or diploma.

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ABSTRACT

The present study confers the biological and chemical quality of groundwater and municipal water of Devarakonda region, Telangana State, for irrigational and drinking purposes. Most of the population depends on groundwater for their daily needs especially for drinking, house needs and irrigation purposes. For this reason, groundwater of Devarakonda were collected and analyzed for pH, electrical conductivity, total dissolved solids (TDS), alkalinity, color, turbidity, total hardness (TH), Iron as Fe, chloride (Cl^-), sulphate (SO_4^{2-}), fluoride (F^-), calcium (Ca^{2+}), magnesium (Mg^{2+}), sodium (Na^+), potassium (K^+), total bacterial count, coliforms, and coliforms. And fifteen groundwater samples were collected and analyzed for pH, electrical conductivity, total dissolved solids (TDS). The physical, chemical, and biological parameters of groundwater in the study area were analyzed and then correlated with those of World Health Organization Standards. The assessment of groundwater samples were carried out to study incrustation and corrosives in areas and also indicate that they can be used for drinking, farming and industrial purposes except for few locations which exceed the permissible limits.

KEY WORDS: Groundwater quality, Devarakonda, Drinking, Irrigation.

1. INTRODUCTION

Water is an important part of our environment and it is a natural resource for sustaining life and environment. In recent times, huge population growth, intense urbanization, increasing industries and tremendous agricultural activities all over the world have contributed to tremendous increase in demand for freshwater for household applications, agricultural and industries [1][2]. Due to insufficient supply of surface water, most of the people in arid and semiarid regions in India are depending primarily on groundwater for their daily needs and irrigation usages. Moreover, groundwater today accounts for a whopping 62.4% of net

irrigation needs, 85% of rural drinking water needs and 50% of urban water needs [3]. It is estimated that more than 1.5 billion people worldwide rely on groundwater as their chief source of drinking water. Hence, it is concluded that the groundwater is an elixir of life and other hand groundwater resource is facing more problems in recent years including quality aspects especially in arid and semiarid regions. Specifically, agricultural chemicals, such as, fertilizers, pesticides and other metal pollution, make the water unfit for drinking purposes [4]. Therefore, knowledge of hydrogeochemistry of water is very essential to evaluate the water for drinking, irrigation and other needs. Eventually, the quality of groundwater is controlled by many factors such as rainfall, topographic relief, mineral dissolution, mineral solubility, ion exchange, oxidation, reduction, natural and anthropogenic activities such as geological structure and mineralogy of the watersheds and aquifers, the residence time, poor sanitary conditions, application of fertilizers and pesticides for higher crop yields without understanding the chemical characteristics of soils and industrial development without following any appropriate remedial measures [5]. Therefore, it is most essential to monitor the quality of water resources in arid and semiarid regions in India particularly groundwater, which is considered as a principal source for drinking and irrigation purposes.

There are number of studies that have been conducted on groundwater quality assessment in many parts of the arid and semiarid regions. Kaur et al. have studied the groundwater quality for drinking and irrigation purposes in Malwa region [6], Punjab. Subramani et al have studied groundwater quality and its suitability for drinking and agricultural use in Tamil Nadu [7]. Sakram et al. have studied groundwater quality and its suitability for drinking and agricultural use in crystalline rocks of Mothkur region, Telangana State, South India [8].

Eventually, Nalgonda district represents a true picture of hard terrain, where there is no sufficient surface water; therefore, most of the district people depend on groundwater for their daily needs. Devarakonda region is one of the mandal in Nalgonda district, where people rely

on groundwater and observed tremendous increase day by day and with number of water quality issues in various places in this region. In few of the areas of Devarakonda, Krishna water supply is available. Devarakonda region is selected to evaluate the groundwater quality issues with main objective to assess the groundwater quality for drinking and irrigation purposes and correlated with WHO standards.

1.1 Geology of the study area

The geology of the area (Fig.1) in general comprises of rocks and mountains of Nalgonda district is one of the 33 districts of Telangana state, with a total geographical area of 1,12,077 sq. km . It has a total population of 350.04 lakhs [9]. The Devarakonda division has 22 Gram Panchayats, 104 revenue villages and 31 mandals [10]. For Administrative convenience the district is divided into 3 revenue divisions located at Nalgonda, Miryalguda and Devarakonda. The district lies between North latitude area 16.693514, 78920197 forms a part of major basin of Krishna river and discovered by survey they connected with road and telecommunications in the district and division. There were 11 Large and Medium scale industries in Devarakonda division. The division is endowed with minerals like stone, clay, building materials and rocks and lime stone have been discovered in Pedda Adiserlapalli mandal area. As for the agriculture is concerned the main source of irrigation is groundwater being 72.56% of total gross irrigated, whereas surface water irrigation accounts for 27.33% of gross area [11].

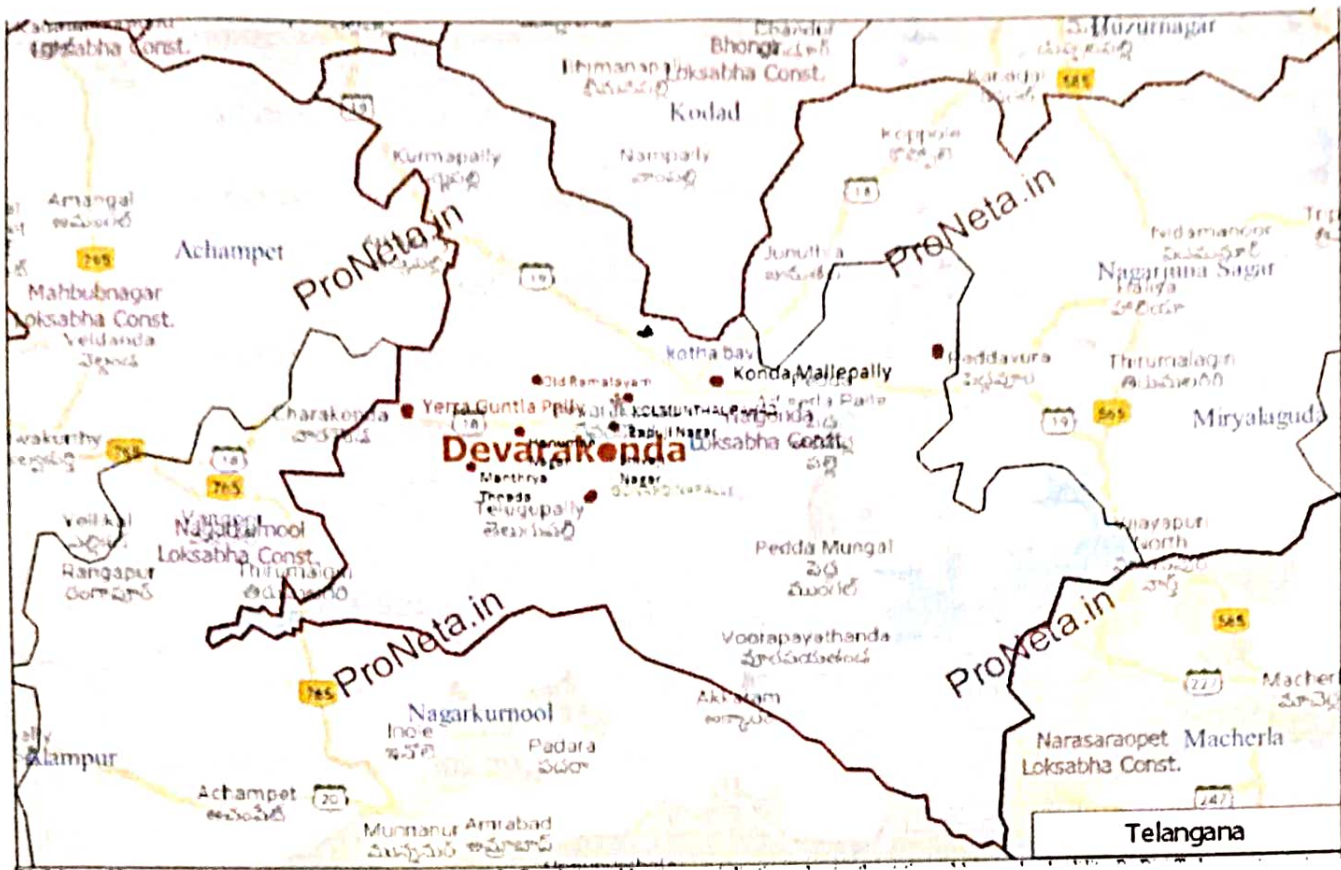


Fig.1. Ground water samplings locations map of Devarakonda region, Telangana, India.

The region predominantly comprise of rocks and in the north-central and south-east parts. In the western and south-west part, the water levels are found between 10 to 20 m. More than 20 m depth range was found as isolated patches in central and western parts of the district. Majority of the area shows rise in the range of 2 -4 m. Majority of the area shows rise in the range of 2 - 4 m. the normal annual rainfall of the state is 939 mm of which Southwest monsoon (June - September) contributes 80% (749 mm), Northeast monsoon (October - December) contributes 13% (120 mm), winter contributes 1% (12 mm) and summer contributes 6 % (58 mm) of the rainfall map of Telangana state.

Groundwater and municipal water samples of Devarakonda were collected and analyzed for pH, electrical conductivity, total dissolved solids (TDS), alkalinity, color, turbidity, total hardness (TH), Iron as Fe, chloride (Cl^-), sulphate (SO_4^{2-}), fluoride (F^-), calcium (Ca^{2+}), magnesium (Mg^{2+}), sodium (Na^+), potassium (K^+), total bacterial count, ecoliforms, and coliforms. And

fifteen groundwater samples were collected from borewells and analyzed for pH, electrical conductivity, total dissolved solids (TDS). The physical, chemical, and biological parameters of groundwater in the study area were analyzed and then correlated with those of World Health Organization Standards. For each individual borewell, no major differences were found in ions concentration among samples collected from different depths during summer seasons, while slight variation was observed for samples taken from different wells.

2. AIMS & OBJECTIVES:

- By analyzing the water sample of the region of Devarakonda, want to understand the quality of water used by the people of this region.
- The data is used to calculate the water quality index which aids in assessing the quality of groundwater, can help taking necessary steps to regular monitoring.
- This data would be useful for the researchers, government, and non-governmental organizations to adopt effective planning methods and mitigation measures and aids in the sustainable development of groundwater.
- The purpose of water level data analysis is for measurements of depth of water level and it give an overall idea regarding the ground water level in the state.
- The water level fluctuation during a particular month of measurement with reference to the decadal mean for the same months gives an idea of the behavior of the ground water level on long-term basis.

3. MATERIALS AND METHODS

Extensive review of literature was done on various methods of water quality analysis. The samples were collected in and around Devarakonda region, Nalgonda district, Telangana, in one

liter polyethylene bottles and stored at 10 °C. All containers used for sampling were washed with 10% nitric acid solution followed by double distilled water. Immediately after sampling, pH and electrical conductivity (EC) were measured in the field with using pH/EC/TDS meter (Hanna HI9811-5). Total hardness (TH) bicarbonate (HCO_3^-), chloride (Cl^-), sulphate (SO_4^{2-}), calcium (Ca^{2+}), magnesium (Mg^{2+}), sodium (Na^+) and potassium (K^+) were analyzed with using standard methods [12]. Analyzed water samples precision expressed as per cent relative standard deviation was below 10%, which is within the acceptable limit [13]. Instrumental, titrimetric and calculation methods were used for water quality analysis are presented in Table 1.

Table 1 Instrumental, titrimetric and calculation methods used for chemical analysis of water samples in Devarakonda region, Telangana State.

Parameters	Characteristics	Analytical method	Reagents	Units
General	pH	p ^H meter	-	-
	Electrical Conductivity	Conductometer	-	μS/cm
	Total dissolved solids(TDS)	TDS meter	-	mg/L
	Total hardness (as CaCO_3)	EDTA titrimetric	EDTA, ammonia buffer and Eriochrome Black-T (EBT) indicator	mg/L
Cations	Calcium (Ca^{+2})	EDTA titrimetric	EDTA, Sodium hydroxide and murexide	mg/L
	Magnesium (Mg^{+2})	Calculation	$\text{MgH}=\text{TH}-\text{CaH}$;	mg/L

			$Mg = MgH \times \text{Eq. Wt of Mg} \times \text{normality of EDTA}$	
	Sodium (Na^+)	Flame photometric	Sodium chloride (NaCl) and KCl	mg/L
	Potassium (K^+)	Flame photometric	Sodium chloride (NaCl) and KCl	mg/L
Anions	Bicarbonates (HCO_3^-)	Titrimetric	Hydrosulphuric acid (H_2SO_4), phenolphthalein and methyl orange	mg/L
	Chloride (Cl^-)	Titrimetric	Silver nitrate (AgNO_3), potassium chromate	
	Fluoride (F^-)	ISE (ion selective electrode; Thermo Orion)	TISAB III and NaF	mg/L
	Sulphates (SO_4^{2-})	UV-visible spectrophotometer	HCl, ethyl alcohol, NaCl, barium chloride, sodium sulphate	mg/L
Biological	Coli	Plate method	Culture medium plate	-
	Ecoli	Plate method	Culture medium plate	-
	Total bacterial count	Plate method	Culture medium plate	-

Standard experimental procedures taken from reference [12] and [17].

4. RESULTS AND DISCUSSION

Different tests were performed under various quality parameters to check the Bore wells. The details of the data which are given in the **Table 2**. Water samples of bore-wells were collected from mentioned sampling stations using standard sampling procedure. The samples were collected during summer season. In order to give the general picture of the municipal water and groundwater, analytical results are presented in **Tables 2 and 3**. The pH values groundwater of the study area varied from 7.04 to 7.67, indicating marginally alkaline nature. The obtained electrical conductivity (EC) values of groundwater samples varied were ranged from 540 to 822 μ . Mhos/cm. Concentration of total dissolved solids (TDS) in groundwater ranged from 122 to 922 mg/L. However, Freeze and Cherry (1979) categorized water on the basis of TDS concentration into four groups which are represented as fresh (TDS < 1000 mg/L), brackish (> 1000 mg/L), saline (>10,000 mg/L) and brine (100,000 mg/L) [14] **Table 4**. Based on this classification, groundwater fall in fresh category. The TH in municipal water and groundwater ranges from 148 to 300 mg/L. The TH classification according to Sawyer and McCarty [15] is clearly illustrated in **Table 5**, and based on this most of the surface and groundwater samples fall in moderate hard and hard category, which is not useful for drinking purposes. Water quality index (WQI) was determined from the physicochemical parameters like P^{H} , Electrical conductivity, TDS, total hardness, total alkalinity, sodium, potassium, calcium, magnesium, chloride, nitrate, sulphate, and fluoride. These results are examined with reference to the drinking water quality standards laid down by WHO (World Health Organisation) [16].

Table 2. Physical, chemical, biological characteristics of groundwater (GW) and municipal water (MW) of the Devarakonda region, Telangana State, South India.

Parameters	Bore Well water	Municipal Tap water	Desirable potable limits as per IS 10500
Dissolved Oxygen (mg/l)	6.2	6.5	6.50
Alkalinity to methyl orange as CaCO ₃ (mg/l)	288	100	<200
Alkalinity to phenolphthalein as CaCO ₃ (mg/l)	Nil	Nil	-
Non-Carbonate Hardness as CaCO ₃	12	48	Not specified
Calcium as CaCO ₃	168	84	<187
Magnesium as CaCO ₃	132	64	<123
Sodium as CaCO ₃	105	119	Not specified
Potassium as CaCO ₃	04	03	Not specified
Sulphate as CaCO ₃	5918	69	<208
Nitrate as CaCO ₃	07	03	<36
Flouride (mg/l)	0.32	0.24	<1.00
Total silica as SiO ₂	5.6	4.1	Not specified
Iron as Fe	0.02	0.02	<0.3
Color	Hazen	Colorless	Colorless
Turbidity	1.30	1.20	<5.0
Chloride (mg/l)	95	98	<352
Total Hardness as CaCO ₃ (Total)	300	148	<300

Electrical Conductivity (μ . Mhos/cm)	818	540	-
pH	7.04	7.67	6.50-8.50
Total Dissolved Solids (ppm)	532	351	<500
Coli forms	04	Nil	<10
Ecoliforms	Absent	Absent	Not specified
Total Bacterial count	390	160	Not specified

The presence of significant counts of coli form bacteria in the bore well water sources is indicative of microorganisms in the water. Sanitary inspection is used to identify the causes of contamination and the risks of future contamination. The turbidity of water is an important parameter as it contributes to the aesthetics of water and leads to its acceptance or rejection for human consumption.

In bore well water dissolved solids are high (532 mg/l). Alkalinity is also high (288 mg/l). Magnesium quantity is 132 mg/l (normal range is below 123). Sulphates are very high i.e 5918 mg/l (normal range is less than 208 mg/l).

All the parameters of Municipal water are correlated with normal range and suitable for drinking water. From the values, interestingly corporation water seems very good for drinking and other human use. The bore well water seemed a bit advisable for washing or any other purposes though will never be recommended for drinking.

Table 3: P^H, Electric conductivity, TDS Values of Different samples in and around Devarakonda.

Sample	Name of the area from which sample is collected and depth of the bore well.	p ^H (WHO value 6.5 to 8.5)	Electric conductivity (WHO value (400µ.mhos/cm.)	TDS (WHO value 300ppm)
GW1	Peddavoora (80fts)	7.08	820	122
GW2	Devarakonda (250fts)	7.02	818	818
GW3	Gonaboinapally (150fts)	7.1	817	618
GW4	Yerraguntapally (250fts)	7.04	818	602
GW5	Yerraguntapally 2 (500fts)	7.02	819	183
GW6	kotha bavi (170fts)	7.1	817	755
GW7	Bapuji nagar DVK (160fts)	7.02	818	666
GW8	Old ramalayam Dvk (350fts)	7.1	816	896
GW9	Shivaji nagar (Dvk) 200fts	7.09	821	796
GW10	Dvk central (400fts)	7.08	819	878
GW11	Kondamallepally (200fts)	7.02	818	919
GW12	Mangalthanda (160fts)	7.05	816	411
GW13	Kolmuthal pahad (180fts)	7.09	814	475
GW14	Ganesh nagar Dvk(300fts)	7.1	813	662
GW15	Hanumannagar Dvk (250fts)	7.06	822	904
GW16	MKR Govt degree college premises	7.04	818	532
MW17	Municipal water	7.67	540	351

GW-01-Peddavoora, GW-02-Devarakonda, GW-03-Gonaboinapally, GW-04-Yerraguntapally 1, GW-05- Yerrakuntapally 2Dvk, GW-06-kotha bavi, GW-07- Bapuji nagar

DVK, GW-08- Old ramalayam Dvk GW-09- Shivaji nagar Dvk, GW-10- Dvk central, GW-11- Kondamallepally, GW-12- Mangalthanda, GW-13- Kolmuthal pahad, GW- Ganesh nagar Dvk, GW-15- Hanumannagar Dvk, Yerraguntapally2, Hanumannagar Dvk, GW-16- MKR Govt Degree College, Devarakonda and MW 17-Municipal water. These areas were the lowest surrounding area the minimum value of TDS is 122 the maximum value of TDS is 919 the average value of TDS is 602.333.

Table 4. TDS classification of groundwater samples.

TDS (mg/l)	TDS (mg/l)
<1000	Fresh
> 1000 mg/L	brackish
> 10,000 mg/L	saline
100,000 mg/L	brine

Table.5. Classification of groundwater based on Electrical Conductivity.

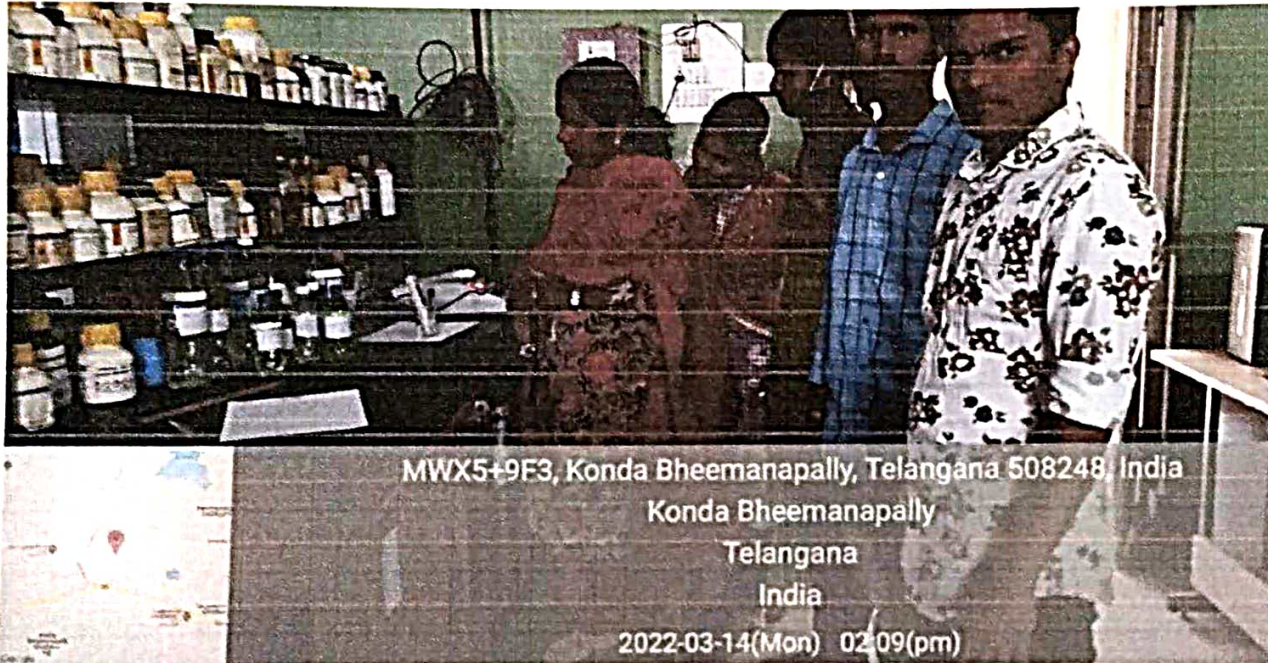
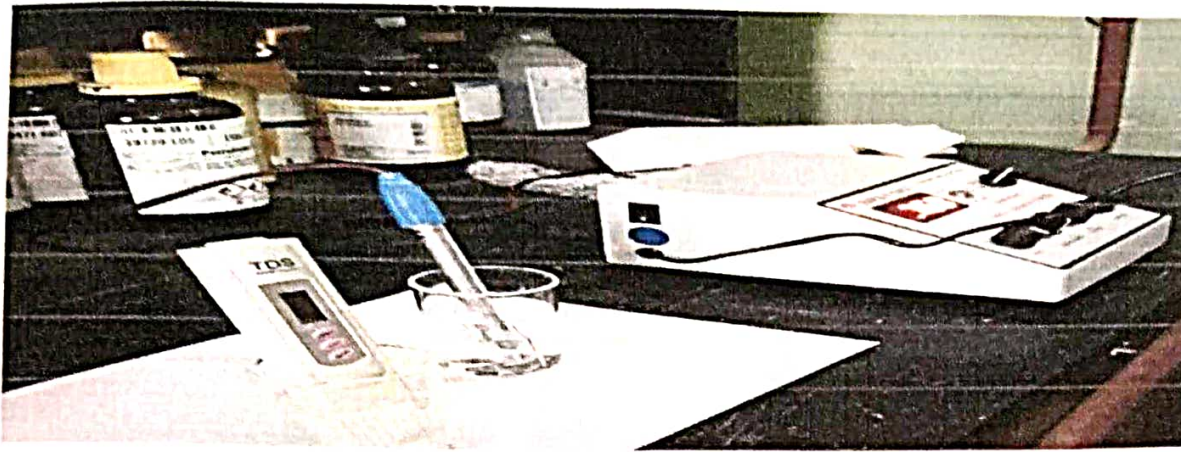
Electrical conductivity	Salinity class	Sample falling in different %
0-250	Low	00
251-750	Medium	5.8
751-2250	High	94.2
2251-6000	Very High	00

5. CONCLUSION

The bore well water is of course not advisable for drinking, can be used for washing or any other purposes. These findings demonstrate the need to come up with source water protection strategies for rural communities where water treatment is not available. To this end, keeping the water sources safe by properly constructed fences, regular maintenances and supervisions of water sources and proper disposal of human and animal wastes are recommended. It was concluded that drinking water sources need to be routinely treated and monitored to eliminate the possible threats to both human and animal health. The present study for fluoride analysis in and

around Devarakonda shows the water samples can be used for drinking, farming and industrial purposes except for few locations which exceed the permissible limits. that all the surrounding areas of devarakonda division according WHO the Ph value of water is to be 6.5 to 8.5 so according to who this 15 areas like peddavoora, devarakonda , gonaboinapally yerrakuntapally1, yerrakuntapally2, kothabavi , bapujinagar, Old ramalayam Dvk, Shivaji nagar Dvk, Dvk central, Kondamallepally, Mangalthanda, Kolmuthal pahad, Ganesh nagar Dvk, HanumannagarDvk, this water is suitable for drinking, the minimum ph value is 7 and the maximum ph value is 8 the average pH value is 7.13 also according to WHO Electric conductivity (WHO value (400 μ S/cm.) and the surrounding 15 areas were the lowest ec values the minimum ec value is 1.113 the maximum ec value is 1.121 the average value of ec is 1.115929 according to who the TDS (WHO values 330ppm Devarakonda, Gonaboinapally, Yerraguntapally 1, kotha bavi, Bapuji nagar DVK, , Old ramalayam Dvk, Shivaji nagar Dvk, Kondamallepally, Ganesh nagar Dvk, Hanumannagar Dvk, This areas were the highest tds values surrounded areas Mangalthanda, Kolmuthal pahad this two areas were nearer to the who value of tds Peddavoora, the TDS of the groundwater suggest that it was classified as fresh water for many samples in the basin drinking and irrigation purposes. The Fluoride (F⁻) concentration varies from 1 - 5 mg/l in groundwater during summer season.

Pictures during experiments in the chemistry lab of Mkr Government Degree College Devarakonda



REFERENCES

- [1]. Adimalla N, Venkatayogi S (2018) Geochemical characterization and evaluation of groundwater suitability for domestic and agricultural utility in semi-arid region of Basara, Telangana State, South India. *Appl Water Sci* 8(1):44. <https://doi.org/10.1007/s13201-018-0682-1>.
- [2]. Alexakis D, Tsakiris G (2010) Drought impacts on karstic spring annual water potential. Application on Almyros (Heraklion Crete) brackish spring. *Desalin. Water Treat.* 16:1–9
- [3]. Raju KCB (1998) Importance of recharging depleted aquifers: state of the art of artificial recharge in India. *J Geol Soc India* 5:429–454.

- [4]. Kelly WR (1997) Heterogeneities in ground-water geochemistry in a sand aquifer beneath an irrigated field. *J Hydrol* 19:154–176.
- [5]. Wang H, Jiang X-W, Wan L, Han G, Guo H (2015) Hydrogeochemical characterization of groundwater flow systems in the discharge area of a river basin. *J Hydrol* 527:433–441.
- [6]. Kaur T, Bhardwaj Renu, Arora Saroj (2016) Assessment of ground water quality for drinking and irrigation purposes using hydrochemical studies in Malwa region, southwestern part of Punjab. *Appl Water Sci, India*. <https://doi.org/10.1007/s13201-016-0476-2>.
- [7]. Subramani T, Elango L, Damodarasamy SR (2005) Groundwater quality and its suitability for drinking and agricultural use in Chitar River Basin, Tamilnadu, India. *Environ Geol* 47:1099–1110.
- [8]. G. Sakram · Narsimha Adimalla (2018), Hydrogeochemical characterization and assessment of water suitability for drinking and irrigation in crystalline rocks of Mothkur region, Telangana State, South India. *Applied Water Science* (2018) 8:143 <https://doi.org/10.1007/s13201-018-0787-6>.
- [9]. <https://www.telangana.gov.in/About/State-Profile>.
- [10]. <http://www.onefivefive.com/india/villag/Nalgonda/Devarakonda>.
- [11]. http://cgwb.gov.in/District_Profile/Telangana/Nalgonda.pdf.
- [12]. APHA (1995) Standard methods for the examination of water and wastewater, 19th edn. American Public Association, Washington, DC.
- [13]. Domenico PA, Schwartz FW (1990) Physical and chemical hydrogeology. Wiley, New York, pp 410–420.
- [14]. Freeze RA, Cherry JA (1979) Groundwater. Prentice-Hall, Englewood Cliffs.
- [15]. Sawyer CN, McCarty PL (1967) Chemistry for sanitary engineers, 2nd edn. McGraw-Hill, New York
- [16]. World Health Organization (2004) Guidelines for Drinking Water Quality. 4th Edition, Geneva.
- [17]. Plate method. <https://food.r-biopharm.com/news/microbial-count-efficient-microbiological-analyses/>

In silico ADME, Bioactivity and Toxicity prediction of some selected Anti viral drugs.



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THE PROJECT REPORT SUBMITTED TO MAHATMA GANDHI UNIVERSITY THE
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PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE DEGREE OF
UNDER GRADUATION IN CHEMISTRY IN CHEMISTRY

JULY-2022



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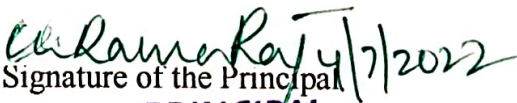
Principal (FAC)

CERTIFICATE

This is to certify that the following mentioned students of Munagala Kondal Rao Govt. Degree College Devarakonda Nalgonda (Dt) have done this group project in chemistry with title '*In silico* ADME, Bioactivity and Toxicity prediction of some selected Anti viral drugs' under the supervision of Dr. M. Alivelu, Assistant professor of Chemistry of this college and submitted the same to the department of Chemistry.

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Date: 07/07/2022


Signature of the Principal
PRINCIPAL
MKR Govt. Degree College
DEVARAKONDA, NALGONDA DIST

DECLARATION

We the students of Munagala Kondal Rao Govt. Degree College are hereby declare that we have done this original research project our selves under the guidance of Dr. M. Alivelu, Asst. Professor of Chemistry, MKR, Govt. Degree College, Devarakonda. We declare that the work incorporated is original and same has not been submitted elsewhere for any degree or diploma.

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ABSTRACT

ADME profiles and bioactivity results of 2-deoxy D-glucose (1), Hydroxy chloroquine (2), and Favipiravir (3) compounds were calculated. Drug likeness criteria based on the rules of Lipinski and Veber appraise that the compounds have classic physicochemical and pharmacokinetic properties to be a good candidate for drug orally.

1. INTRODUCTION

Viruses are major pathogenic agents causing a variety of serious diseases in humans, other animals, and plants. Viruses are one of the most widespread of all organisms and are capable of infecting every species of animal from mammals down to insects, plants, and even bacteria. It seems there are more species of viruses in the world than of all other creatures put together. The deadliest, most horrifying diseases the world has ever seen have been initiated by viruses.

The COVID-19 is the one among them and the name given to the 2019 novel corona virus [1]. Formerly, six corona viruses (Coves) are recognized to cause diseases in humans, and these can be defined as low, highly pathogenic Coves [2]. According to the World Health Organization (WHO), the WHO China Office reported pneumonia of unknown etiology in Wuhan City at the end of 2019 [3]. The Chinese authority of the health showed that the patients primarily tested negatively for the viruses and respiratory bacteria but later tested positive for a new corona virus. The virus was presently isolated and its genome sequenced by Chinese scientists. In February 2020, the corona virus disease 2019 was selected as the disease COVID-19 by WHO. The COVID-19 can cause infections in different animals and most infections of the respiratory tract in individuals, including the Middle East respiratory syndrome (MERS) and severe acute

respiratory syndrome (SARS). The COVID-19 virus is completely different from the viruses accountable for SARS and MERS [4]. The COVID-19 genome sequences got from the patient's part a 79.5% sequence related to that of SARS-Cove. The signs and symptoms characteristically occur among two weeks after contact and consist of fever, coughing, respiratory disorders, pain in the chest, and trouble breathing. Possibly deadly complications include pneumonia and kidney failure [5]. As on December 30, 2020, a total number of 82,739,879 cases of COVID-19 (with 1,804,879 deaths) have been reported from 191 countries worldwide according to the WHO situation report. United States of America as epicenter of the current COVID-19 reported maximum deaths associated with COVID-19 (20,034,309 laboratory confirmed cases with 347,713 deaths). The countries where more than 2,000,000 people are affected include India (10,264,426), Brazil (7,577,890), Russia (3,131,550), France (2,600,498), England (2,432,888), Turkey (2,194,272) and Italy (2,083,689). In the present development, the United States of America and most European nations bear the brunt of the burden of illness and death associated with COVID-19 relative to other nations. The latest increase in consistently reported patients with COVID-19 has now reached acute care stocks, restricting acute care coverage to just a limited percentage of critical patients. This may also have led to the elevated fatality ratio found during the COVID-19 outbreak.

In abundant recent works, 2-DG, Hydroxychloroquine, Favipiravir has been designed for experimental treatments of COVID-19, in which it has been recommended as a helpful drug for the purpose [6]. Computer-aided drug design (CADD) has recently been utilized successfully in drug discovery.

On May 8, 2021, the Drugs Controller General of India approved an oral formulation of 2-deoxy-D-glucose for emergency use as adjunct therapy in moderate to severe corona virus patients. The drug was developed by the DRDO along with Dr. Reddy's Laboratories, who jointly claimed via a press release, that the drug "helps in faster recovery of hospitalized patients and reduces supplemental oxygen dependence"[7]. The Wire as well as the Hindu noted that the approval was based on poor evidence; no journal publication (or preprint) concerning efficacy and safeties are yet available

2-deoxy D-glucose (Fig.1) has been used as a targeted optical imaging agent for fluorescent *in vivo* imaging. In clinical medical imaging (PET scanning), fluorodeoxyglucose is used, where one of the 2-hydrogens of 2-deoxy-D-glucose is replaced with the positron-emitting isotope fluorine-18, which paired gamma rays, allowing distribution of the tracer to be imaged by external gamma camera(s). This is increasingly done in tandem with a CT function which is part of the same PET/CT machine, to allow better localization of small-volume tissue glucose-uptake differences.

Hydroxychloroquine (Fig.1) is a quinoline medicine used to treat or prevent malaria, a disease caused by parasites that enter the body through the bite of a mosquito. Malaria is common in areas such as Africa, South America, and Southern Asia. Hydroxychloroquine is not effective against all strains of malaria, or against malaria in areas where the infection has been resistant to a similar drug called chloroquine. Hydroxychloroquine is also used to treat symptoms of rheumatoid arthritis and discoid or systemic lupus erythematosus.

Favipiravir (Fig.1) is an antiviral medication with a pyrazine structure that was developed by the Fujifilm group in Japan and has an action against a wide range of RNA viruses [8]. It has been

more over- examined for different types of influenza in the last years .In abundant recent works, Favipiravir has been designed for experimental treatments of COVID-19, in which it has been recommended as a helpful drug for the purpose.

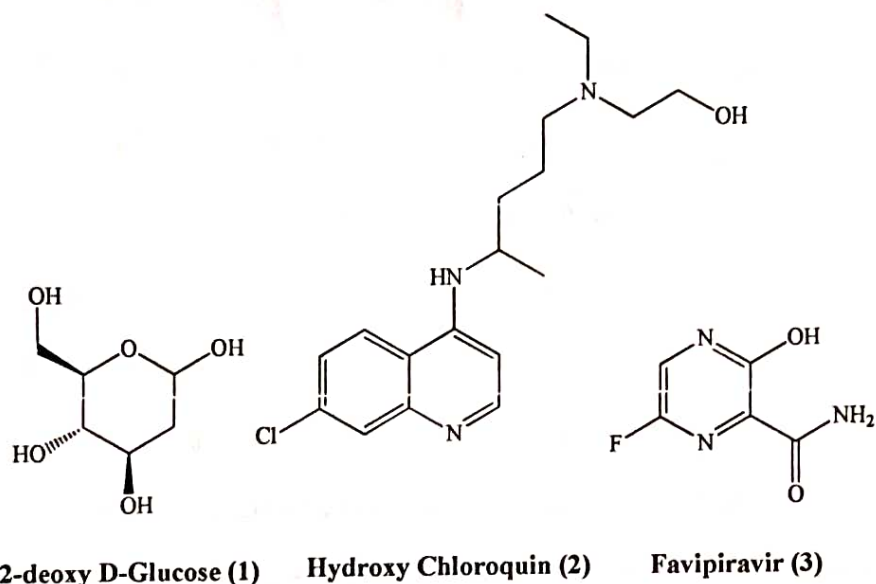


Fig 1. Structures of 2-deoxy D-Glucose, Hydroxy chloroquin, and Favipiravir.

In general, there are different approaches used together in CoVID-19 treatment, and in these approaches, drug compounds can be selected according to virus-based and host-based treatment [9]. The first process offers broad-spectrum antiviral drugs, previously used to treat viral infections by typical assays. These drugs' effects on pseudo corona viruses, cytopathic, viral production, and living cells plaque formation can be measured in these approaches. This method contains interferon I and interferon II. These drugs have pharmacodynamic and pharmacokinetic features with their drug regimens and side effects. On the other hand, the anti-COVID-19 virus has no specific effects and can be related to extreme opposite reactions. The third process includes the publication of a chemical library with various compounds or databases containing knowledge about the properties of transcription for different cell lines .This process may provide

fast and high yields for many simply obtainable compounds and then estimate them with an antiviral test. Several drugs with significant immunological and physiological effects such as kinase signal transduction, an estrogen receptor, DNA synthesis or repair, lipid, and protein metabolism have been recognized in these drug reuse programs [10]. The fourth process also includes treatment methods used by Acupuncturists with a meaningful result in the management of patients with COVID-19. One hypothetically effective method is a synthetic form of quinine, called hydroxyl chloroquine. Presently, malaria is treated with natural and synthetic forms of the Chinese herbal medicine Qing Hao. On the other side, Cortegiani et al. found that chloroquine appears to be effective in reduced the replication of COVID-19 in vitro. Furthermore, Gao et al. showed that chloroquine is significantly effective compared to a control group in 100 patients for symptoms duration, decreasing pneumonia exacerbations, and viral clearance postpone. Also, this study displayed that chloroquine might decrease the length of hospital stays. Chloroquine and oxygen treatment is recommended by the Infectious and Tropical Disease Society and the Dutch Centre for Disease Control in Italy, with separate dosage guidelines compared with the Chinese Protocol. Colson et al. conclude that sufficient preclinical indication is available for the chloroquine used in COVID-19 treatment. In 2003, Chinese medicine had been used in the same disorders during the SARS outbreak, with recognized clinical successes. Despite primary clinical achievements and hopeful research, the treatment rate for COVID-19 remains difficult to succeed. The herbal formula Qing Fei Pai Du Tang had a reply rate of 90 percent of a total of 214 clinical cases of COVID-19 related pneumonia, with respect to the National Administration of Traditional Chinese Medicine. Patients were treated in the provinces of Shanxi, Hebei, Shanxi, and Heilongjiang during this clinical research. A description of the response rate of 90% is as follows: symptoms changed dramatically in around 60% and the remaining 30% stable.

Another research surveyed 701 COVID-19 patients in Ten Chinese Cities who received Qing Fei Pai Du Tang medication. A total of 130 patients (18.5%) were cured, symptom changes were achieved in a further 268 patients (38.2%), and recovery occurred in 212 patients (30.2%). Other studies showed that Lian Hua Qing Wen Capsule decreased the COVID-19 symptoms and upgraded healing. Besides, the Lianhuaqingwen Capsules and Shu Feng JieDu Capsules have played a significant role in treating infectious diseases like influenza A (H1N1). Conversely, the safety and effectiveness of these drugs in COVID-19 require to be more validated via clinical tests. Furthermore, nucleoside analogs may have numerous action mechanisms, including chain termination, lethal mutagenesis, and nucleotides' biosynthesis inhibition. The tribavirin and favilavir are nucleoside analogs representatives, which pooled with Avigan and oseltamivir in acute influenza care are superior to oseltamivir only. On the other hand, the Neuraminidase inhibitors such as zanamivir and oseltamivir are suggested as antiviral treatment in infection. The oseltamivir has been commonly used for COVID-19 in China. The chiefly point for patients is the beginning of antiviral medication immediately after disease initiation. It has revealed that neuraminidase inhibitors are more active in MERS-CoV infection, but there is no significant indication that oseltamivir is influential in COVID-19 care. Moreover, Remdesivir may be the possible drug for the care of COVID-19. The experiments in animals exhibited that effectively decrease the virus titer of mice infected with COVID-19 comparing to healthy mice, decrease the damage of the lung tissue. Conversely, the safety and efficiency of Remdesivir in patients with COVID-19 still need more clinical research. Presently, other types of drugs have been starting to be influential in vitro, like fusion peptides, RNA synthesis inhibitors, and anti-inflammatory drugs. In Turkey, in the first Covid-19 cases encountered, it was taken into account the accumulation of experiences and treatment protocols of China, previously living the process of

combating the pandemic. But after the first 1-2 weeks, Turkey has developed its treatment algorithm based on its own clinical observation and experience. Furthermore, the Ministry of Health also made updates to the algorithm according to the developments within the framework of the recommendations of the Scientific Board established after the Corona virus outbreak. In Turkey, a dissociated and effective treatment protocol was formed differently from other applications in the world. The strategies developed in the light of the objective recommendations of the Scientific Committee based on scientific data, the professional experience of healthcare professionals who implement these strategies, their organizational capabilities, well-equipped and extensive hospital infrastructure and the capacity of intensive care units with high-quality equipment above the world average was formed a great advantage in combating Covid-19. Since the Ministry of Health has sufficient drug stocks, Hydroxychloroquine treatment was started at the early stage of the disease. Favipiravir treatment was started when replicating the virus, that is, before the disease gets seriously worse, before the need for intensive care. Whereas in the first applications, it was started in the intensive care process, this is an application that has been put into practice in the intensive care stage of the disease in many countries still, but it is thought that it is not very effective at this stage. It was given up from early intubation (invasive ventilation) in intensive care patients. Because it was observed that this did not change the course of the disease much. Noninvasive ventilation technique (continuous positive pressure airway (CPCA)) has begun to be used instead of invasive ventilation, which is insufficient. Thus, the risks of lung damages caused by invasive ventilation were also prevented. It was also observed that the disease was not a typical ARDS table as described, additional problems such as coagulopathy (coagulation disorder) also occurred, and patients were also lost due to this reason. Accordingly, anticoagulant drugs have also affixed the algorithm. For the diagnosis of Covid-19, the capacity

of quantity and quality of IL, present in hospitals in Turkey, more effective than PCR, has increased its capability for rapid diagnosis. In the cure of Covid-19 patients in Turkey, the following protocols were applied after grouping patients. Mild, possible/definitive Covid-19 outpatient case treatment; Hydroxychloroquine and oseltamivir therapy was recommended for 5 days period for patients with mild symptoms, under 50 years of age, pneumonia and concomitant hypertension, cardiovascular diseases, chronic airway disease, diabetes, cancer, immune suppression and patients with undiagnosed/influenza . Moderate, possible/definitive Covid-19 service treatment; it was recommended to azithromycin addition for 5 days to Hydroxychloroquine and oseltamivir therapy for the cure of patients , who need hospitalization, but do not have a pneumonia picture and clinic heavy and do not have accompanying co morbid diseases, and the cases in the middle clinic . Serious, possible/definitive Covid-19 case treatment; it was recommended to use favipiravir for 5 days, which is an effective antiviral in the management of patients with acute pneumonia, concomitant co morbid diseases, and severe clinic, and to add favipiravir to the treatment of patients who worsen the clinic while taking Hydroxychloroquine treatment in cases of mild disease, and develop pneumonia. The following suggestions can be made for treatments in some special cases by the experience gained during the treatments in Turkey. According to clinical, laboratory, and radiological findings, among those who started Covid-19 treatment, it is known that it is appropriate to add drugs such as quinoline to the effective atypical agents' beta-lactam antibiotics to those who are considered to have infection/pneumonia. Inhaler drugs that should be given with nebulizer should be administered with a metered-dose inhaler due to the risk of transmission. In non-invasive mechanical ventilation (NIMV) applications, the mask should be preferred for reducing infectious. It is recommended to evaluate the option of follow-up without treatment if the

symptoms/clinic are mild, if co morbid conditions are not accompanied in pregnant women with Covid-19 definitive diagnosis, to use treatment Lopinavir 200 mg/ritonavir 50 mg tb 2x2 10/14 days orally and to add Hydroxychloroquine 5 days depending on the situation. Favipiravir should not be used in nursing mothers and pregnant women. There is concern about the use of non-steroidal anti-inflammatory drugs (NSAIDs). This concern has evolved because several young patients used NSAIDs in the early phase of the disease, and their condition deteriorated. However, currently, there is insufficient data to support NSAID use or to ban it altogether. For suspicious cases, acetaminophen should be preferred as an analgesic and antipyretic. In all Covid-19 patients who are hospitalized for the prevention of venous thromboembolism, prophylaxis is recommended using low molecular weight heparin if there are no contraindicated conditions such as active bleeding and severe thrombocytopenia. In intensive care patients whose clinic worsens while lying in the service, the addition of steroid 1-2 mg/kg/day 5-7/day and high dose of vitamin C, 25 g/day, according to the clinical condition of the patients, the addition of IL-6 inhibitor tocilizumab in patients with cytokine storm findings, should be evaluated. Immune plasma therapy and stem cell therapy have been begun to use as promising treatments in patients whose general condition has deteriorated and did not respond to treatment. Since SARS-CoV-2 is a newly encountered virus, no vaccine, monoclonal antibody, or a drug that directly affects it has been developed yet. Although there are promising studies on vaccine and drug development, there is a high probability of not being completed for this pandemic period. Therefore, one of the fastest and easiest treatment options that first come to mind and can directly target SARS-CoV-2 is to take serum or plasma from people who have survived this disease and are considered to contain antibodies against this virus and use it for both preventive and therapeutic purposes. Serum or plasma treatment has started to be easier and find application area by increasing the

number of those who survived the disease. Unlike the vaccine, this use falls into the class of passive antibody therapy (PAT) and includes benefits and risks. Considering the previous experience with plasma treatment, it seems to be the only available treatment option for the Covid-19 pandemic in today's conditions where vaccines and drugs could not be developed. One of the most important factors in the positive outcome of this treatment can be summarized as the presence of sufficient neutralizing antibodies in the transplanted plasma, and another is the rapid start of treatment of individuals with potential risk factors such as age. Briefly, since the recovered patients' immune systems reacted differently to the virus, treatment should be directed considering the possibility of not having enough antibodies or not at all, if very few. In the treatment to be performed 1 week after the first plasma treatment, it is more appropriate to give the plasma of another donor or the plasma from a few donors to the patient. This is valid for the current situation, but it is expected that an efficacy test will be carried out before it is given for neutralization in the future. The PAT carries several risks. There can also be an enhanced risk of antibody-dependent viral infections, and its molecular mechanism is unknown. Besides, there is another risk that antibody therapy will suppress the development of acquired immunity. While this situation requires that the antibody level in the treatment of PAT is sufficient until the disease is completely eliminated, it should be considered that an immune memory cannot be formed due to the metabolism of the externally given antibodies. Consequently, the vaccine should be taken into account after PAT. In addition, the duration of the plasma antibody and the duration of effectiveness of this acquired immunity are also important as additional information. In this pandemic era, it is expected to pay attention to the vaccination of individuals who are not yet immune, rather than vaccinating individuals who have naturally active antibody counts. It is not known how it will affect the people who got and survive this disease in the long term. The

'COVID-19 Patient Monitoring Center' was opened by the Istanbul Medical Faculty to answer these questions. This center will investigate whether the coronavirus causes permanent damage in patients by performing various tests and examinations on those who got coronavirus and survive. While struggling with this disease, some problems were observed in organs such as the lungs, heart, intestines, and liver. Some publications were started to be discussed in the literature; some question marks whether these problems will continue, especially whether lung, liver, or kidney problems will be carried in the long term. Thereupon, 'COVID-19 Patient Monitoring Center' was established in Turkey, and this center is the first center in Turkey and the world for this goal. For patients who have had severe COVID-19 infection, some problems that may occur by following them at 1, 3, 6, 9, and 12th months after their treatment will be diagnosed and treated at this center.

2. METHODOLOGY

Computer-aided drug design (CADD) has recently been utilized successfully in drug discovery. This method requires substantially less effort, time, and money when compared to traditional approaches. The use of computational technology for identifying the new candidate drugs help to reduce the number of experimental studies and for improving the success rate. For this reason, we used the ADMET (adsorption, distribution, metabolism, excretion and toxicity) profile for a measure of pharmacokinetics parameters of the three compounds proposed by the Pre-ADMET server, to evaluate their chances to become a candidate drug in the future. Computational techniques were applied to analyze the various physiochemical features Pharmacokinetic descriptors which were calculated for the 1-3 compounds through the online tool Molinspiration Cheminformatics server [11] (<http://molinspiration.com/>). ADMET SAR2 [12] was used to

predict the absorption, distribution, and metabolism and toxicity properties of the selected compounds. SwissADME webserver was used to investigate the oral bioavailability properties of the compounds.

3. RESULTS AND DISCUSSION

In silico pharmacokinetics ADMET and drug likeness prediction

The Drug similarity is the excellence concept used for a drug like property, which is explained as a complex equilibrium of different molecular properties and structural characteristics that determine whether a particular molecule is similar to known drugs. These molecular properties are mainly hydrophobicity, electronic distribution, hydrogen bonding properties and the existence of severally pharmacological characteristics that influence the molecular exploit of organisms, as well as bioavailability, transport properties, interaction with proteins, reactivity, toxicity, metabolic stability, and many others. Lipinski's rule of five was used to determine the bioavailability of bulk materials to examine the drug-likeness properties. This rule plays a major role in drug discovery. In the present study, the physiochemical properties analysis of molecules was carried out with the Molinspiration Cheminformatics program, drug-likeness of the 1-3 molecules was calculated and it is presented in Table 1. The study good membrane permeability of molecules should obey the following: H-bond donors (HBD) were found in-between 1-3 (≤ 5), H-bond acceptors (HBA \AA^2) were found to be 3-5 (≤ 10), all 1-3 molecules partition coefficient ($M_i \log P$) is less (≤ 5), molecular weight is also less than ($\leq 500 \text{g/mol}$), Vander Walls topological polar surface area (TPSA) value is $48.38 - 90.15 \text{\AA}^2$ ($\leq 120 \text{\AA}^2$) [13]. So, the compounds obeys Lipinski's rule of five for all cases.

Table 1. Drug likeness prediction of 1-3 compounds using molinspiration online tool.

Compound:	1	2	3
Molecular formula:	C ₆ H ₁₂ O ₅	C ₁₈ H ₂₆ ClN ₃ O	C ₅ H ₄ FN ₃ O ₂
Molecular weight (g/mol):	164.16	321.85	157.10
milog P:	-1.95	3.98	-0.52
TPSA(Å ²)	90.15	48.38	89.11
No. of H bond acceptor:	2	4	5
No. of H bond donor:	1	2	3
No. of rotatable bonds:	1	8	1
No. of violations	0	0	0
Rule of five violations	0	0	0

Topological polar surface area (TPSA).

The bioactivity score of the compounds 1-3, Ion channel modulator, kinase inhibitor, nuclear receptor ligand, protease inhibitor, and enzyme inhibitor values are given in Table 2.

Table 2. Bioactivity score of 1-3 compounds.

Parameter		1	2	3
Bioactivity	GPCR Ligand	-0.52	0.31	-0.43
	ICM	-0.13	0.16	0.42
	KI	-0.84	0.33	-0.35
	NRL	-0.78	-0.23	-1.14
	PI	-0.34	0.04	-0.58
	EI	0.69	0.00	-0.18

GPCRL: G protein-coupled receptor ligand; ICM: Ion channel modulator;

KI: Kinase inhibitor; NRL: Nuclear receptor ligand;

PI: Protease inhibitor; EI: Enzyme inhibitor.

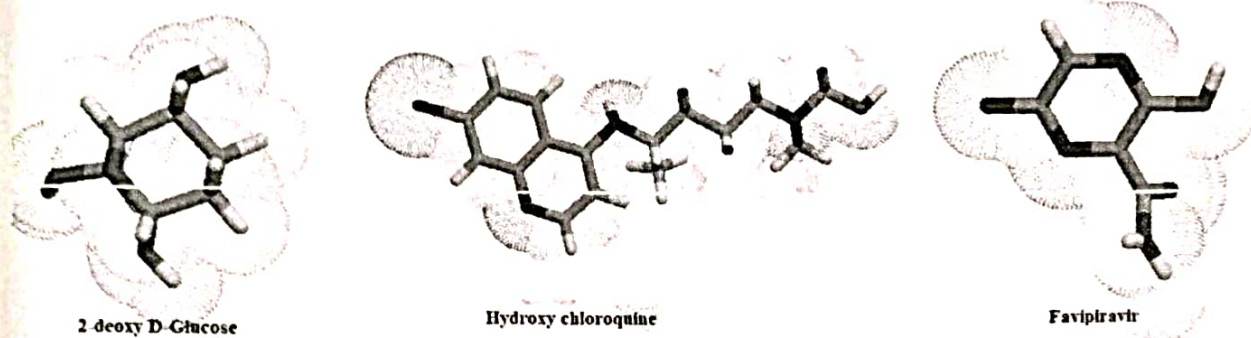


Fig 2: Stable conformations of compounds 2-deoxy D-Glucose (1), Hydroxy chloroquine (2), and Favipiravir (3).

Table 3. ADMET prediction of 1-3 compounds.

Properties	Compound 1	Compound 2	Compound 3
AlogP98	-1.747100	3.457400	-0.182000
Surface area	63.849	136.659	60.697
Adsorption			
Pure water solubility (mg/L)	930297	224.786	13724.8
Buffer solubility (mg/L)	283303	12.9119	195.055
Caco-2 permeability	7.70057	46.0839	17.0145
P _{gp} inhibition	Non	Non	Non
Skin permeability	-4.98488	-3.08546	-4.43154
Human-Intestinal adsorption (%)	62.522	88.049	100
Distribution			
BBB permeability(log BB)	0.0987037	2.28794	0.25861
VD _{ss} (human, log L/kg)	-0.232	1.021	-0.262
CNS permeability	-3.6	-2.654	-3.037
Fraction unbound	0.898	0.286	0.737
Metabolism			
CYP 2C19 inhibition	Inhibitor	Non	Inhibitor
CYP 2C9 inhibition	Inhibitor	Non	Inhibitor
CYP 2D6 inhibition	Non	Inhibitor	Non
CYP 2D6 substrate	Non	Substrate	Non
CYP 3A4 substrate	Weakly	Weakly	Non
CYP 3A4 inhibition	Non	Non	Non
HIA	41.652679	94.660945	72.7553
MDCK	0.583686	45.1085	1.66307

Plasma protein binding	42.018589	88.996812	3.519089
SKlogD-value	-1.784380	2.058490	-0.75472
SklogP-value	-1.784380	3.622950	-0.75472
SklogS-buffer	0.236990	-4.415190	-2.90603
SklogS-pure	0.753360	3.174410	-1.05868
Excretion			
Total clearance (log ml/min/kg)	0.611	1.096	0.861
Renal OCT2 substrate	No	No	No
Toxicity			
Algae at	0.195245	0.0108916	0.233301
Ames test	mutagen	mutagen	mutagen
Carcino-Mouse	negative	negative	negative
Carcino-Rat	negative	negative	positive
Daphnia-rat	15.7025	0.0554527	1.66438
hERG-inhibition	low risk	medium risk	low risk
Medaka-at	210.661	0.00582202	3.15729
Minnow -at	93.6604	0.00995439	1.2034
TA100 -10RLI	negative	negative	negative
TA100 -NA	positive	negative	positive
TA1535-10RLI	negative	negative	positive
TA1535-NA	negative	negative	positive

MW (molecular weight (g/mol)), log P (partition coefficient), colon cancer cell line (Caco-2), N_{rot} (number of rotatable bonds), Fsp3 (fraction Csp3), N_{vio} (number of violations by the Lipinski and Veber drug-likeness criteria), HIA (human intestinal absorption), Caco-2 (human adenocarcinoma colon cells), BBB (blood-brain barrier penetration), Pgp (P_1 glycoprotein substrate), bioactivity by the GPCR (G-protein coupled receptor), ICM (ion channel modulator), kinase inhibitor, nuclear receptor ligand, protease inhibitor and enzyme inhibitor models and toxicity by the acute oral model.

The oral bioavailability and other physicochemical properties of the selected compounds and standards obtained using the SwissADME web tool. The bioavailability radar (Fig. 3) gives a swift catch sight of the important physicochemical properties and drug-likeness of the selected compounds [14]. As shown in (Fig. 3), the colored portion (Pink) shows the most desirable area for each of the bioavailability properties (LIPO, SIZE, INSOLU, POLAR, INSATU, and FLEX). Surprisingly, all the selected compounds and standards were in the colored region. According to Lipinski rule of five (RO5), the SIZE (Molecular Weight) of a good drug candidate is expected not to be more than 500gmol⁻¹, of which of all selected compounds (1-3) obey). The INSOLU (insolubility) requirement of the selected compounds and standards as depicted in their ESOL

(Log S) and ESOL Class revealed that compounds 1-3 are very soluble. All the selected compounds fall within the INSATU recommended range of values and have the best oral bioavailability since all their physicochemical properties fall within the optimal colored (pink) region.

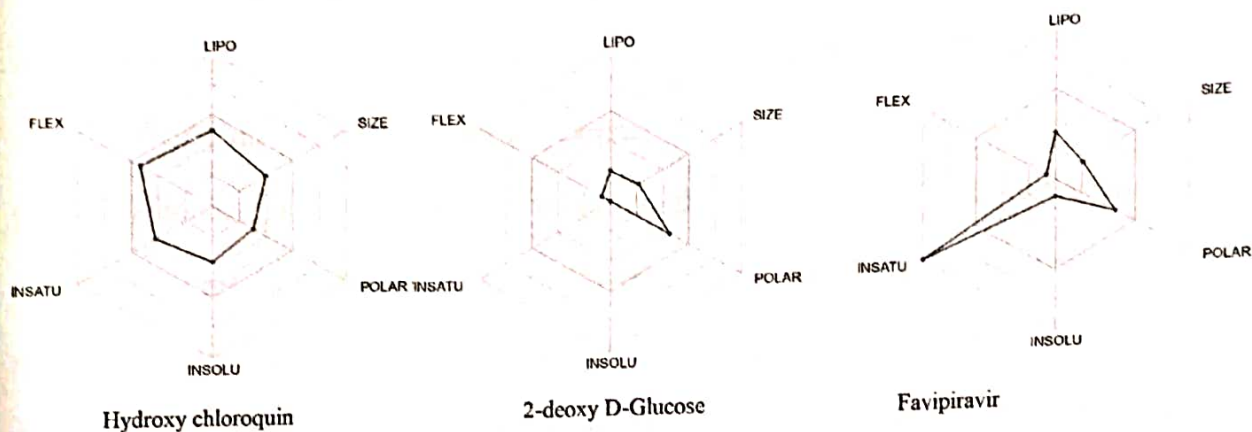


Fig.3: The bioavailability radar for the selected compounds. Pink area = Most desirable area for each of the bioavailability properties, LIPO = Lipophilicity, POLAR = Polarity, INSOLU = Insolubility, FLEX = Flexibility, SIZE = Molecular weight, INSATU = Unsaturation

In silico ADMET (absorption, distribution, metabolism, excretion, and toxicity) screening of drug could avoid the tremendous cost and time associated with the in vivo experiments, and attracted more and more attention. As shown ADMET properties in Table 3, three compounds exhibited positive results for blood brain barrier (BBB) criteria i.e. they can pass through BBB, possess good human intestinal absorption value and Hydroxy chloroquine show high BBB value. All the 1-3 compounds are non-carcinogenic and showed safer category acute oral toxicity. So, they are relatively harmless and safe for oral administration. The three compounds showed inhibition to the P-glycoprotein inhibitor where, the inhibition can interrupt the absorption, permeability and retention of the compounds. Inhibition of the potassium channels by human ether-a-go-related gene (hERG) mainly generate QT syndrome-leading to fatal ventricular

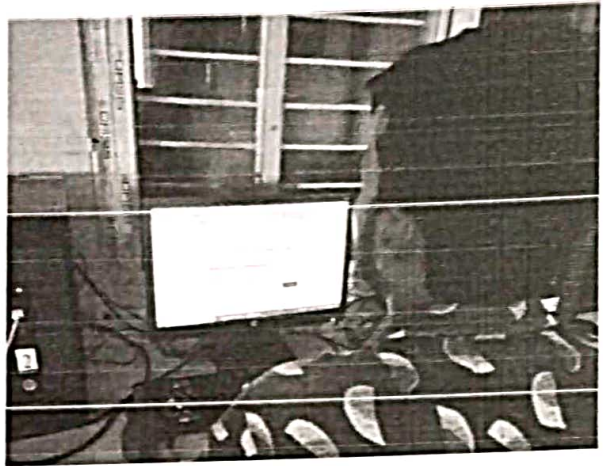
arrhythmia [10], and need to withdraw many drugs from pharmaceutical market. In the present study, three compounds showed weak inhibitory feature towards human hERG and hence comparatively safer. For metabolism, all compounds were predicted to be No Inhibitor for CYP450 3A4, which meant that they might be metabolized by CYP 3A4. In addition, all compounds might not inhibit CYP450 1A2 isoform, but they might inhibit CYP450 3A4 isoform. Based on the predicted total clearance rate, liver and kidney tissue could be used to clear all compounds in combination. The expected toxicity indicated that all compounds might be harmful to the liver and that none of them caused skin irritation and mutagenicity. All design molecules with synthetic accessibility scores showed lower structural complexity, thus demonstrating synthetic feasibility (Table 3). Computational pharmacokinetic and toxicological studies and accessible synthetic methods indicated that virtually designed compounds could be used as lead compounds for further development. Overall the ADMET results ensure the good drug-likeness properties and hence could be potent new possible candidate for better performance.

4. CONCLUSION

Scientists are working hard to determine the new corona virus's characterization and develop antiviral therapies and vaccines. However, the virus's pathogenesis is still not fully known, and new studies are needed in this regard. Currently, the only way to prevent the spread of Covid-19 is an effective infection control method. The most appropriate treatment for patients under observation diagnosed with Covid-19 is still unknown. Therefore, treatment protocols should be followed within the framework of existing health rules some vaccines have been developed, and the prophylactic drug has not yet been developed, although intensive trials are ongoing for both.

Although some vaccines have been developed for the COVID-19 corona virus, intensive work is still being done to develop specific drugs or vaccines. Computational pharmacokinetic and toxicological studies and accessible synthetic methods indicated these 1-3 compounds could be used as lead compounds for further development. Overall the ADMET results ensure the good drug-likeness properties and hence could be potent new possible candidate for better performance.





REFERENCES

- [1]. Cascella, M.; Rajnik, M.; Cuomo, A.; Dulebohn, S.C.; Di Napoli, R. Features, Evaluation and Treatment Coronavirus (COVID-19). Stat Pearls [Internet], Stat Pearls Publishing 2021.
- [2]. Zhu, N.; Zhang, D.; Wang W.; Li X.; Yang B.; Song J. A novel coronavirus from patients with pneumonia in China, 2019. *N Engl J Med* 2020, 382, 727-733, <https://doi.org/10.1056/NEJMoa2001017>.
- [3]. Corman, V.M.; Landt, O.; Kaiser, M.; Molenkamp, R.; Meijer, A.; Chu, D.K.W. Detection of 2019 novel coronavirus (2019-nCoV) by real-time RT-PCR. *Eurosurveillance* 2020, 25, 2000045, <https://doi.org/10.2807/1560-7917.ES.2020.25.3.2000045>.
- [4]. Zu, Z.Y.; Jiang, M.D.; Xu, P.P.; Chen, W.; Ni, Q.Q.; Lu, G.M. Coronavirus disease 2019 (COVID-19): a perspective from China. *Radiology* 2020, 296, E15-E25, <https://doi.org/10.1148/radiol.2020200490>.
- [5]. Sanders, J.M.; Monogue, M.L.; Jodlowski, T.Z.; Cutrell, J.B. Pharmacologic treatments for coronavirus disease 2019 (COVID-19): a review. *Jama* 2020, 323, 1824–36, <https://doi.org/10.1001/jama.2020.6019>.
- [6]. What is 2-deoxy-D-glucose (2-DG) and is it effective against Covid?, *The Economic Times*, 17 May 2021.
- [7]. Jump up to:^{a b} *Koshy, Jacob (2021-05-11). "Questions remain on DRDO's COVID dru in silco study.*
- [8]. Y. Furuta, BB. Gowen, K. Takahashi, K. Shiraki,DF. Smee, DL. Barnard, Favipiravir (T-705), a novel viral RNA polymerase inhibitor, *Antivir.Res.* 100 (2) (2013) 446-454, <https://doi.org/10.1016/j.antiviral.2013.09.015>.
- [9]. Cao, B.; Wang, Y.; Wen, D.; Liu, W.; Wang, J.; Fan, G. A trial of lopinavir–ritonavir in adults hospitalized with severe Covid-19. *N Engl J Med* 2020, 382, 1787-1799, <https://doi.org/10.1056/NEJMoa2001282>.
- [10]. Zhou, Y.; Hou, Y.; Shen, J.; Huang, Y.; Martin, W.; Cheng, F. Network-based drug repurposing for novel coronavirus 2019-nCoV/SARS-CoV-2. *Cell Discov* 2020, 6, 14, <https://doi.org/10.1038/s41421-020-0153-3>.

- [11]. C. A. Lipinski, F. B. W. Lombardo, B. W. Dominy, P.J. Feeny, "Experimental and computational approaches to estimate solubility and permeability in drug discovery and development settings," *Advanced Drug Delivery Reviews* 23 (1997): 3-25.
- [12]. Cheng F, Li W, Zhou Y, Shen J, Wu Z, Liu G, Lee PW, Tang Y. admetSAR: a comprehensive source and free tool for assessment of chemical ADMET properties. 2012;52: 3099–3105.
- [13]. Zhao, J.; Liao, X.; Wang, H.; Wei, L.; Xing, M.; Liu, L. Early virus clearance and delayed antibody response in a case of COVID-19 with a history of co-infection with HIV-1 and HCV. *Clin Infect Dis* 2020, <https://doi.org/10.1093/cid/ciaa408>.
- [14]. Daina A, Zoete V. A boiled-egg to predict gastrointestinal absorption and brain penetration of small molecules. *ChemMed₁ Chem*. 2016;11:1117–21.

FIELD WORK SUBMITTED

To

**THE CHEMISTRY DEPARTMENT,
MKR GOVERNMENT DEGREE COLLEGE, DEVARAKONDA**

On

“DETECTION OF FOOD ADULTERANTS”



Supervised by

Dr. M. ALIVELU

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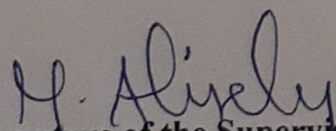
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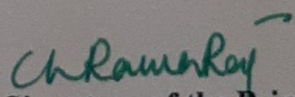
DEVARAKONDA

CERTIFICATE

This is to certify that the following mentioned students of MKR Govt. Degree College, Devarakonda, Nalgonda (dt) have done the group project in Chemistry with title: **'DETECTION OF FOODADULTERANTS'** under the supervision of Dr. M. Alivelu, Assistant professor of Chemistry of this college and submitted the same to the department of Chemistry, MKR GDC Devarakonda.

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1. INTRODUCTION:

The Objective of this project is to study some of the common food adulterants present in different food stuffs.

Adulteration in food is normally present in its most crude form; prohibited substances are either added or partly or wholly substituted. Normally the contamination/adulteration in food is done either for financial gain or due to carelessness and lack in proper hygienic condition of processing, storing, transportation and marketing. This ultimately results that the consumer is either cheated or often become victim of diseases. Such types of adulteration are quite common in developing countries or backward countries. It is equally important for the consumer to know the common adulterants and their effect on health.

The increasing number of food producers and the outstanding amount of import foodstuffs enables the producers to mislead and cheat consumers. To differentiate those who take advantage of legal rules from the ones who commit food adulteration is very difficult. The consciousness of consumers would be crucial. Ignorance and unfair market behavior may endanger consumer health and misleading can lead to poisoning. So we need simple screening, tests for their detection. In the past few decades, adulteration of food has become one of the serious problems. Consumption of adulterated food causes serious diseases like cancer, diarrhea, asthma, ulcers, etc. Majority of fats, oils and butter are paraffin wax, castor oil and hydrocarbons. Red chilli powder is mixed with brick powder and pepper is mixed with dried papaya seeds. These adulterants can be easily identified by simple chemical tests.

Several agencies have been set up by the Government of India to remove adulterants from food stuffs. Selection of wholesome and non-adulterated food is essential for daily life to make sure that such foods do not cause any health hazard. It is not possible to ensure wholesome food only on visual examination when the toxic contaminants are present in ppm level. However, visual examination of the food before purchase makes sure to ensure absence of insects, visual fungus, foreign matters, etc.

1.1 SOME ADULTERANTS IN COMMON FOOD

Majority of adulterants used by the shopkeepers are cheap substitutes easily available. For example, adulterants in fats, oils and butter are paraffin wax, castor oil and hydrocarbons. Red chili powder is mixed with brick powder, turmeric powder is mixed with yellow lead salts and pepper is mixed with dried papaya seeds. Similarly sugar is contaminated with washing soda and other insoluble substances, milk is adulterated with starch, argemone oil is used to adulterate mustard oil, vanaspati ghee is mixed with deshi ghee, beson is mixed with khesari dal etc. These type of adulterants makes a food stuff inferior.

1.2 IMPACT OF ADULTERANTS

Every day we hear and watch live on television sets how the food items are being adulterated and this spurious, unhygienic and harmful food is entering our houses. We have seen how milk and milk products are being made from urea, soap and other harmful chemicals. We all know that vegetables are being given injections to make them grow faster and overnight. The other day we saw how steroids were being injected to chickens to make them into a hen in a very short span of time. We have also come across evidence as to how the fruits are being ripened with the use of harmful chemicals.

Adulteration of food causes several health problems in humans. Some of the health hazards include stomach ache, body ache, anemia, paralysis, and increase in the incidence of tumors, pathological lesions in vital organs, abnormalities of skin and eyes. Hence food adulteration should be given great importance due to its effect in the health significance of the public. The people are suffering from heart disease, kidney failure, skin diseases, asthma and other chronic diseases. The people are hapless victims of this adulteration industry running in full swing and unchecked.

1.3 DIFFERENT CHEMICAL TESTS FOR DETECTION OF ADULTERANTS

Food adulteration has now become a burning problem. The adulterants used are so similar to natural foodstuffs that it becomes very difficult for a common man to detect them. A few simple tests can be done to detect adulterants found in common foodstuffs.

Metanil yellow in pulses:

Shake 5 gms of the suspected pulses with 5 ml of water. Add a few drops of hydrochloric acid. A pink colour shows the presence of metanil yellow.

Kesari Dal in Chana or Other Dals:

Add 5 ml of normal hydrochloric acid to a small quantity of dal in a glass. Keep the glass in simmering water for 15 minutes. Development of pink colour indicates the presence of Kesari dal. By visual detection-shape of dal. The kesari dal is wedge shaped.

Water in milk:

Measure the specific gravity with a lactometer. The normal values will fall between 1.030 and 1.034. Milkmen are wise to the test and may dilute the milk only to the right density, so this is only a rough test.

Starches in milk:

Add a drop of iodine solution to a small quantity of milk. Milk containing starch turns blue. Pure milk turns a coffee shade.

Vanaspati in pure ghee:

Take about one teaspoonful of melted butter with an equal quantity of concentrated hydrochloric acid in a test tube. Add 2 or 3 drops of furfural solution. Shake it well for one minute and let it stand for five minutes.

Appearance of pink colour in the lower layer of acid means that vanaspati is present in pure ghee/butter as an adulterant.

Argemone oil in mustard oil:

Heat the mixture of oils with a little amount of nitric acid for two to three minutes. A red colour will appear if argemone is present.

Chalk or any other dust or dirt in sugar:

Dissolve sugar in water, the impurities will settle down at the bottom. Etc.

2. METHODOLOGY:**2.1 Detection of Starch in Milk**

Along with water, a very common adulterant of milk is starch. Milk consists of three basic components which are water (about 80%), fat (about 3.5%) and solids containing protein, lactose and mineral matters (about 8.5%). Milk is adulterated with starch to maintain the thickness of fat extracted milk or diluted milk. The presence of starch can be detected by adding iodine solution to milk.

Reagent used- Iodine solution or tincture of iodine.

Procedure- At first 5mL of milk sample is taken in a test tube and is boiled for 3-4 minutes. Then it is cooled and 1-2 drops of iodine solution is added to it and is shaken well.

Detection- Appearance of blue colour indicates the presence of starch in the sample.

Table for different samples-

S. NO	SAMPLES	RESULT
1.	Amul TAZA	Adulterant absent.
2.	Diary milk	Adulterant present.
4.	Vijaya Dairy milk	Adulterant absent.

2.2 DETECTION OF YELLOW DYE IN TURMERIC POWDER

Turmeric (haladhi) powder is a popular natural dye used in cooked food. The powder is often adulterated with rice powder, besan, wheat powder etc. which makes the colour of the turmeric pale. To make the colour bright, often lead chromate, which is a poisonous chemical or coal tar dye is added to turmeric powder.

A. DETECTION OF LEAD CHROMATE

Reagents: Con. HCL and 1% Diphenyl carbazide in rectified spirit.

Procedure: 1g of the turmeric powder sample is taken in a test tube and 5ml of concentrated HCL is added to it. The mixture is shaken thoroughly. Now 1ml of 1% diphenyl carbazide reagent is added.

Detection: Appearance of pink to red colour indicates the presence of lead chromate, $PbCrO_4$, in the sample.

B. DETECTION OF COAL TAR DYE

Reagents: Concentrated HCL and petroleum ether (40-60^o C).

Procedure: 5g of the sample is taken in a test tube and 10 mL petroleum ether is added to it. The mixture is shaken vigorously and is allowed to stand. 5 mL of conc. HCL is added and is again shaken thoroughly.

Detection: The aqueous acid becomes pink to red in colour if coal tar is present.

Table for different samples

S.NO.	SAMPLES	RESULT
1.	MDH Haldi powder	Adulterant absent.
2.	Open sample	Adulterant present.
3.	Bharat haldi	Adulterant absent.

2.3. DETECTION OF WASHING SODA, CHALK POWDER AND WATER INSOLUBLE SUBSTANCE IN SUGAR

Chalk powder is a water insoluble substance which is often used as a common adulterant in sugar. Moreover sugar is usually contaminated with washing soda.

Detection of various insoluble substances

Reagent: concentrated H_2SO_4 , alcoholic solution of α -naphthol, dil HCl.

Procedure: A small amount of sugar is taken in a test tube and is shaken it with little water. Pure sugar dissolves in water but insoluble impurities do not dissolve.

Detection: Insoluble substances appear at the bottom of the test tube if they are present.

Detection of chalk powder, washing soda

Reagent: dil. HCl

Procedure: To a small amount of sugar taken in a test tube, a few drops of dil. HCl is added and observed.

Detection: Brisk effervescence of CO_2 shows the presence of chalk powder or washing soda in the given sample of sugar.

Table for different samples

S.NO.	SAMPLES	RESULT
1.	Open sample	Adulterant present.
2.	Packed sample	Adulterant absent.

2.4 DETECTION OF RED COLOURED LEAD SALTS IN CHILLI POWDER.

Chilli powder often adulterated with red are coloured lead salts and brick powders.

Reagents: Dil. HNO_3 , KI.

Procedure: To a sample of chilli powder dil. HNO_3 is added. The solution is filtered and a few drops of potassium iodide solution is added to the filtrate.

Detection: Yellow ppt. indicates the presence of lead salts in chilli powder and insoluble substances indicates the presence of brick powder in the sample.

Table for different samples

S.NO.	SAMPLES	RESULT
1.	Ashirvad Chilli powder	Adulterant present.
2.	Open chilli powder	Adulterant present.

2.5 DETECTION OF KHESARI DAL IN BESON

Beson powder is usually adulterated with khesari dal which contains butyl oxalyl alanine amine (BOAA) which causes lethargy and ultimate paralysis in lower limbs of human body on regular consumption. The detection of BOAA in beson powder indicates adulteration of it with khesari dal.

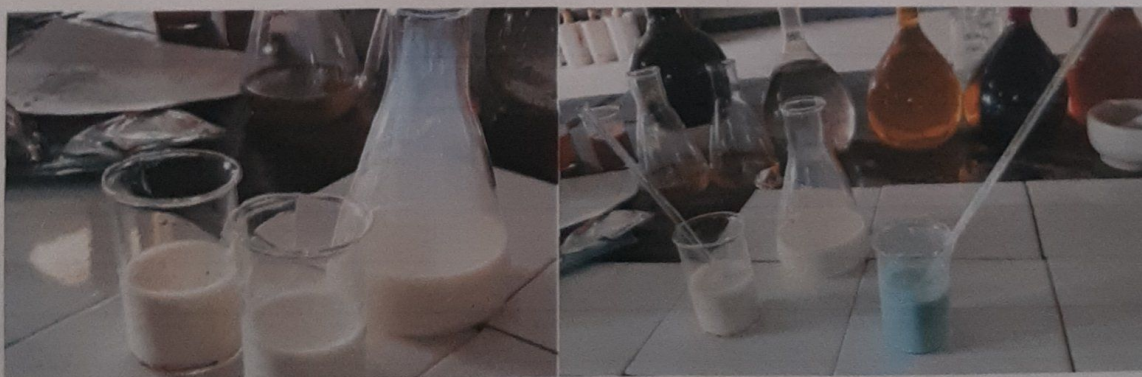
Reagents: dil. HCl.

Procedure: To 1g of the beson sample is taken in a test tube and 10 mL of 70% HCl is added to it. The content is boiled for some time.

Detection: Development of pinkish colour indicates adulteration of bason with khesari dal.

Table for different samples

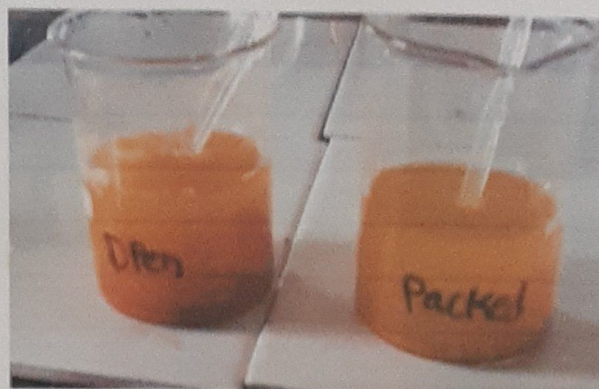
S.NO.	SAMPLES	RESULT
1.	Open sample	Adulterant present
2.	Packed sample	Adulterant present.



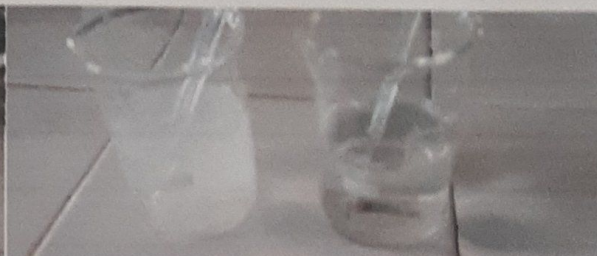
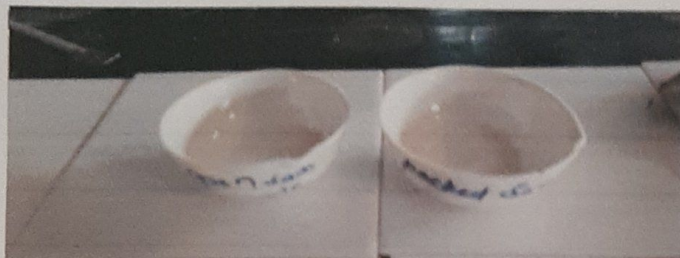
Different milk samples were chemically tested for food adultrants.



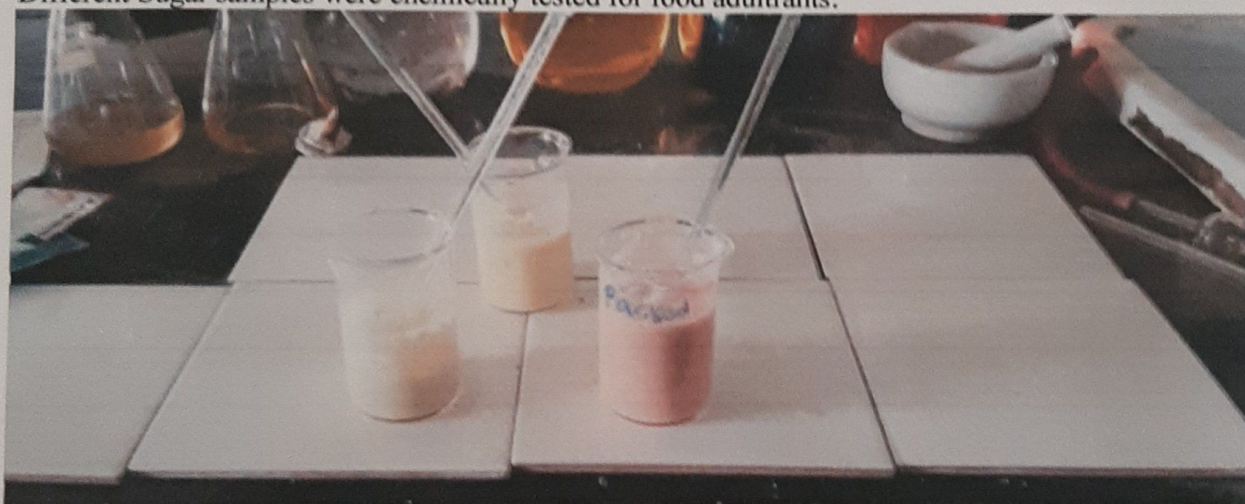
Different Chilli powder samples were chemically tested for food adultrants



Different Haldi powder samples were chemically tested for food adultrants.



Different Sugar samples were chemically tested for food adultrants.



Different Besan samples were chemically tested for food adultrants.



3. CONCLUSION

Different chemical reactions studied involving in the process of detection of different adulterants in different food items. These experiments were performed for the purpose of detecting various adulterants present in common food. The results obtained during these experiments have been shown in this project. The experiments have been performed by common laboratory methods. Packed samples are far better than open samples as in open samples, possibility of contamination with food adulterants is more.

4. Suggestions:

1. At the time of food purchase consumer needs thorough examination and it can be of great help.
2. Label declaration on packed food is very important for knowing the ingredients and nutritional value. It also helps in checking the freshness of the food and the period of best before use.
3. The consumer should avoid taking food from an unhygienic place and food being prepared under unhygienic conditions.
4. It is always better to buy certified food from reputed shop.

REFERENCES:

1. Principles of Inorganic Chemistry by Puri, Sharma and Kalia Vishal Publications 1996.
2. Elements Of Practical Chemistry, SUDARSAN BARUAH, Department of Chemistry, Cotton college, Guwahati.
3. Senior Secondary Practical Chemistry, Dr. KAMALESH CHOUDHURY, Dr. SATYENDRA KUMAR CHOUDHURY, Cotton College Guwahati.