DEVELOPMENT OF Fe/GRAPHENE NANOCATALYST FOR OXYGEN REDUCTION REACTION IN ALKALINE ZINC-AIR AND HYDROGEN-OXYGEN FUEL CELL

Project work

Submitted to Christ College (Autonomous), Irinjalakuda (University of Calicut) in partial fulfilment of the requirements for the award of Degree of BACHELOR OF SCIENCE IN CHEMISTRY

Submitted by

Aleenamol Daison

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CERTIFICATE

This is to certify that the project work entitled "DEVELOPMENT OF Fe/GRAPHENE NANOCATALYST FOR OXYGEN REDUCTION REACTION IN ALKALINE ZINC-AIR AND HYDROGEN-OXYGEN
FUEL CELL" is an authentic work done by Aleenamol Daison (Reg no CCAUSCH001),Anghitha K P (Reg no CCAUSCH002),Christeena M V (Reg no CCAUSCH003),Devika Gopakumar (Reg no CCAUSCH004), Jaladwajan A R (Reg no CCAUSCH005), final semester B.Sc. Chemistry students of this institution under my supervision in partial fulfilment of the requirements for the degree of Bachelor of Science in Chemistry of Christ College (Autonomous), Irinjalakuda (University of Calicut).

Dr.V.T.JOY

Head of the Department of Chemistry
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Place :

Irinjalakuda

Date :

20 April 2023

DECLARATION

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ACKNOWLEDGEMENT

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CHAPTER 1

DEVELOPMENT OF Fe/GRAPHENE NANOCATALYST FOR OXYGEN REDUCTION REACTION IN ALKALINE ZINC-AIR AND HYDROGEN-OXYGEN FUEL CELL

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Project work

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Acknowledgement

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Dissertation submitted to the Christ College (Autonomous) in partial fulfilment of the requirement for the Degree of

BACHELOR OF SCIENCE

IN

CHEMISTRY

Submitted by

SAHAL MALIK M A

Reg. No: CCAUSCH012

2020-2023

P.G AND RESEARCH DEPARTMENT OF CHEMISTRY

CHRIST COLLEGE (Autonomous), IRINJALAKUDA

THRISSUR-680125

DECLARATION

I, **SAHAL MALIK M A** (Reg.No.CCAUSCH012) do hereby declare that, this dissertation work entitled Studies on the physicochemical properties of coconut water submitted to the University of Calicut in Partial Fulfilment of the requirement for the award of degree of Bachelor of Science was carried under the guidance of Dr. DIGNA VARGHESE, Assistant professor, Department of Chemistry, Christ College, Irinjalakuda and it is a record of original project work carried out by me and it has not previously formed the basis for the award of, any degree, Diploma fellowship or other similar title of recognition by any other university or institutions.

Place: Irinjalakuda **SAHAL MALIK M A**

Date: 29th APRIL 2023.

STUDIES ON THE PHYSICOCHEMICAL PROPERTIES OF COCONUT WATER

Bonafide record of work done by

SAHAL MALIK M A [Reg. No.: CCAUSCH012]

Literature review submitted in partial fulfilment of the requirement for the degree

Of

BACHELOR OF SCIENCE

In Chemistry

CALICUT UNIVERSITY

April 2023

Dr. DIGNAVARGHESE
Faculty Guide

……

Dr. V.T.JOY
Head of the Department

Certified that the candidate was examined in the viva voice examination held on

……

(Internal Examiner)

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(External Examiner)

CERTIFICATE

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Studies On The Physicochemical Parameters Of Tender Coconut Water

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IN

CHEMISTRY

Submitted by

SREELAKSHMI K B

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DECLARATION

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Place: Irinjalakuda SREELAKSHMI K B

Date: 29th APRIL 2023.

STUDIES ON THE PHYSICOCHEMICAL PROPERTIES OF COCONUT WATER

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SREELAKSHMI K B [Reg. No.: CCAUSCH013]

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IN

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DECLARATION

I, **V VINEETHA** (Reg.No.CCAUSCH014) do hereby declare that, this dissertation work entitled Studies on the physicochemical properties of coconut water submitted to the University of Calicut in Partial Fulfilment of the requirement for the award of degree of Bachelor of Science was carried under the guidance of Dr. DIGNA VARGHESE, Assistant professor, Department of Chemistry, Christ College, Irinjalakuda and it is a record of original project work carried out by me and it has not previously formed the basis for the award of, any degree, Diploma fellowship or other similar title of recognition by any other university or institutions.

Place: Irinjalakuda V VINEETHA

Date: 29th APRIL 2023.

STUDIES ON THE PHYSICOCHEMICAL PROPERTIES OF COCONUT WATER

Bonafide record of work done by

V VINEETHA [Reg. No.: CCAUSCH014]

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Head of the Department

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Place: Irinjalakuda **AJEENA ANTONY**

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STUDIES ON THE PHYSICOCHEMICAL PROPERTIES OF COCONUT WATER

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Place: Irinjalakuda **ALEENA WILSON**

Date: 29th APRIL 2023.

STUDIES ON THE PHYSICOCHEMICAL PROPERTIES OF COCONUT WATER

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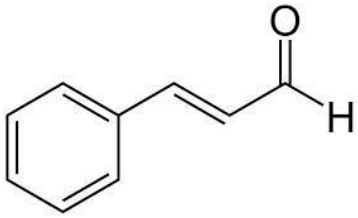

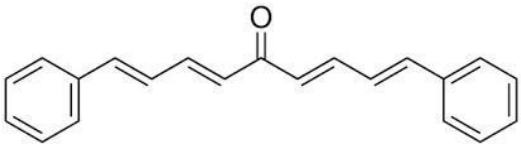

CINNAMALDEHYDE - EXTRACTION FROM CINNAMON, PROPERTIES OF CINNAMON OIL AND PREPARATION OF ALDOL DERIVATIVE FOR SUNSCREEN APPLICATIONS

AMEESHA M.M

CCAUSCH019

CINNAMALDEHYDE – EXTRACTION FROM CINNAMON, PROPERTIES OF CINNAMON OIL AND PREPARATION OF ALDOL DERIVATIVE FOR SUNSCREEN APPLICATIONS

B.Sc. Dissertation Work

AMEESHA M. M
MARCH 2023

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PROJECT REPORT SUBMITTED TO UNIVERSITY OF CALICUT
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DEGREE OF

BACHELOR OF SCIENCE IN CHEMISTRY

By

AMEESHA M M

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29th MARCH 2023

Certificate

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Irinjalakuda,

29th March 2023

Dr. V T Joy,
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IRINJALAKUDA

Dr. Robinson P Ponminiessary,
(Supervising Guide)
Assistant Professor,
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IRINJALAKUDA

DECLARATION

I hereby declare that the work presented in this thesis entitled "CINNAMALDEHYDE – EXTRACTION FROM CINNAMON, PROPERTIES OF CINNAMON OIL AND PREPARATION OF ALDOL DERIVATIVE FOR SUNSCREEN APPLICATIONS" is entirely original and was carried out by me under the supervision of Dr. Robinson P Ponminiessary, Department of Chemistry, Christ College, Irinjalakuda and has not been included in any other thesis submitted previously for the award of any degree.

Irinjalakuda, **ALISHA P.A**

29th March, 2023

Acknowledgement

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ALISHA P.A

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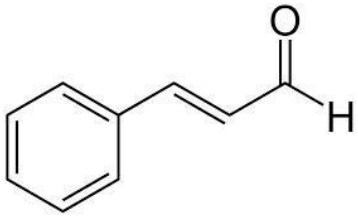

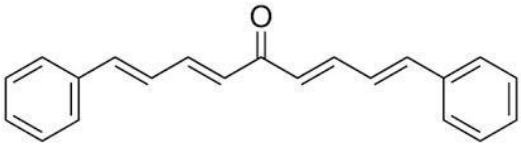

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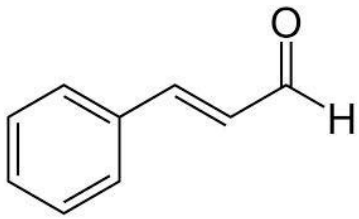

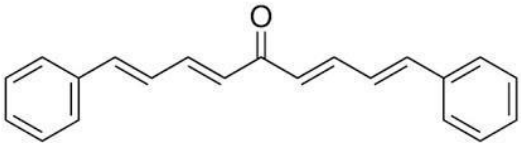

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ARUNIMA M

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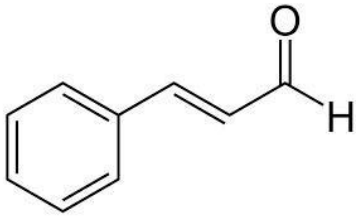

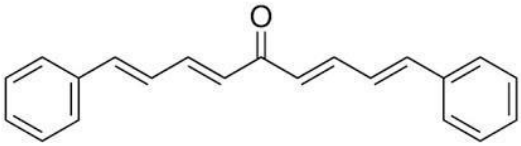

CINNAMALDEHYDE - EXTRACTION FROM CINNAMON, PROPERTIES OF CINNAMON OIL AND PREPARATION OF ALDOL DERIVATIVE FOR SUNSCREEN APPLICATIONS

ASHA PRASAD

CCAUSCH021

CINNAMALDEHYDE – EXTRACTION FROM CINNAMON, PROPERTIES OF CINNAMON OIL AND PREPARATION OF ALDOL DERIVATIVE FOR SUNSCREEN APPLICATIONS

B.Sc. Dissertation Work

ASHA PRASAD
MARCH 2023

CINNAMALDEHYDE – EXTRACTION FROM CINNAMON, PROPERTIES OF CINNAMON OIL AND PREPARATION OF ALDOL DERIVATIVE FOR SUNSCREEN APPLICATIONS

PROJECT REPORT SUBMITTED TO UNIVERSITY OF CALICUT
IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR

DEGREE OF

BACHELOR OF SCIENCE IN CHEMISTRY

By

ASHA PRASAD

Reg: No: CCAUSCH017

DEPARTMENT OF CHEMISTRY
CHRIST COLLEGE
IRINJALAKUDA 680125

29th MARCH 2023

Certificate

This is to certify that the dissertation entitled ***"CINNAMALDEHYDE - EXTRACTION FROM CINNAMON, PROPERTIES OF CINNAMON OIL AND PREPARATION OF ALDOL DERIVATIVE FOR SUNSCREEN APPLICATIONS "*** *is an authentic record of project work carried out by Ms. ASHA PRASAD under my supervision, in partial fulfillment of the requirements for the degree of Bachelor of Science of Calicut University, and further that no part thereof has been presented before for any other degree.*

Irinjalakuda,

29th March 2023

Dr. V T Joy,
Head of Department
CHRIST COLLEGE,
IRINJALAKUDA

Dr. Robinson P Ponminiessary,
(Supervising Guide)
Assistant Professor,
CHRIST COLLEGE,
IRINJALAKUDA

DECLARATION

I hereby declare that the work presented in this thesis entitled "CINNAMALDEHYDE – EXTRACTION FROM CINNAMON, PROPERTIES OF CINNAMON OIL AND PREPARATION OF ALDOL DERIVATIVE FOR SUNSCREEN APPLICATIONS" is entirely original and was carried out by me under the supervision of Dr. Robinson P Ponminiessary, Department of Chemistry, Christ College, Irinjalakuda and has not been included in any other thesis submitted previously for the award of any degree.

Irinjalakuda, **AMEESHA M.M**

29th March, 2023

Acknowledgement

A project work is indeed an outcome of hard work and helps a lot in framing up a person in his/her career. At the outset, I convey my heartfelt gratitude and indebtedness to Prof. Robinson P Ponminiessary, Assistant Professor, Department of Chemistry, Christ College, Irinjalakuda for coordinating and supervising this work. My thanks and gratitude also go to the Head of the Department and all the members of the Chemistry Department, Christ College, Irinjalakuda for their guidance and inspiration given during the B.Sc. career.

AMEESHA M.M

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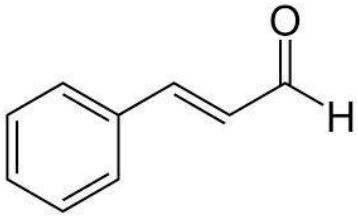

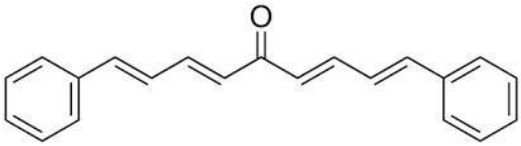

CINNAMALDEHYDE - EXTRACTION FROM CINNAMON, PROPERTIES OF CINNAMON OIL AND PREPARATION OF ALDOL DERIVATIVE FOR SUNSCREEN APPLICATIONS

ASWIN KRISHNA O.R

CCAUSCH022

CINNAMALDEHYDE – EXTRACTION FROM CINNAMON, PROPERTIES OF CINNAMON OIL AND PREPARATION OF ALDOL DERIVATIVE FOR SUNSCREEN APPLICATIONS

B.Sc. Dissertation Work

ASWIN KRISHNA O.R
MARCH 2023

CINNAMALDEHYDE – EXTRACTION FROM CINNAMON, PROPERTIES OF CINNAMON OIL AND PREPARATION OF ALDOL DERIVATIVE FOR SUNSCREEN APPLICATIONS

PROJECT REPORT SUBMITTED TO UNIVERSITY OF CALICUT
IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR

DEGREE OF

BACHELOR OF SCIENCE IN CHEMISTRY

By

ASWIN KRISHNA O.R.

Reg: No: CCAUSCH022

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IRINJALAKUDA 680125

29th MARCH 2023

Certificate

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Irinjalakuda,

29th March 2023

Dr. V T Joy,
Head of Department
CHRIST COLLEGE,
IRINJALAKUDA

Dr. Robinson P Ponminiessary,
(Supervising Guide)
Assistant Professor,
CHRIST COLLEGE,
IRINJALAKUDA

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Irinjalakuda, **AMEESHA M.M**

29th March, 2023

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A project work is indeed an outcome of hard work and helps a lot in framing up a person in his/her career. At the outset, I convey my heartfelt gratitude and indebtedness to Prof. Robinson P Ponminiessary, Assistant Professor, Department of Chemistry, Christ College, Irinjalakuda for coordinating and supervising this work. My thanks and gratitude also go to the Head of the Department and all the members of the Chemistry Department, Christ College, Irinjalakuda for their guidance and inspiration given during the B.Sc. career.

AMEESHA M.M

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ISOLATION AND CHARACTERIZATION OF CONSTITUENTS OF ESSENTIAL OIL FROM GINGER

Project report submitted to the University of Calicut in partial fulfilment of the requirement for the award of the Degree,

BACHELOR IN CHEMISTRY

By

ATHIRA SATHYAN
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DEPARTMENT OF CHEMISTRY,

CHRIST COLLEGE, IRINJALAKUDA (AUTONOMOUS),

THRISSUR, KERALA-680125

APRIL 2023

CANDIDATE'S STATEMENT

I hereby declare that the dissertation entitled, "ISOLATION AND CHARACTERIZATION OF CONSTITUENTS OF ESSENTIAL OIL FROM GINGER" is a genuine record of project work done by me under the guidance of Dr. Titto Varghese, Assistant professor, Department of Chemistry, Christ college (Autonomous), Irinjalakuda and has not been submitted to any university or institution for the award of any degree or diploma.

I further declare that the results presented in this work and consideration made therein contribute to the advancement of knowledge in Chemistry.

Place: Irinjalakuda
Date: 25/04/2023 ATHIRA SATHYAN

ACKNOWLEDGEMENT

Upon the successful completion of this project, I would like to extend my sincere and deepest gratitude to the following without whom the work would not be possible. Primarily I would like to thank God Almighty for being able to complete this project on time and for the favorable circumstances that made it. I wish to express my sincere gratitude to my project guide Dr. Titto Varghese, Assistant Professor, Department of Chemistry, Christ College, Irinjalakuda for his guidance, for providing necessary advice, for his patience in hearing my ideas, and for all the endeavours he took for the completion of this project. Without his enormous support and guidance, this study would not be possible. I extend my thanks to Dr. V.T Joy, Head of the Department of Chemistry, Christ College, Irinjalakuda, and all other teaching and non-teaching staff of the department for their suggestions, comments and encouragement during this work. I am also indebted to Rev. Dr. Jolly Andrews CMI, Principal, Christ College, Irinjalakuda, for providing all the available facilities for this work. Lastly, I would like to thank my family members for their support and effort.

ATHIRA SATHYAN

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ABSTRACT

The objective of this project was to extract the essential oil from ginger (Zingiber officinale) obtained from Kerala using the Hydrodistillation method. The chemical constituents of the essential oil were characterized through UV Spectroscopy and is submitted for Gas Chromatography-Mass Spectrometry (GC-MS).The main components that may be detected in the essential oil of Ginger were **α**-Pinene, Camphene, Beta-Pinene, Beta-Myrcene, Zingiberene, Terpenol, **α**-Farnesene,Nerolidol, Beta-Sesquiphellandrene,Beta-Bisabolene,Citral, etc.

ISOLATION AND CHARACTERIZATION OF CONSTITUENTS OF ESSENTIAL OIL FROM GINGER

Project report submitted to the University of Calicut in partial fulfilment of the requirement for the award of the Degree,

BACHELOR IN CHEMISTRY

By
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APRIL 2023

CANDIDATE'S STATEMENT

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Place: Irinjalakuda
Date: 25/04/2023 KRISHNENDU G

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KRISHNENDU G

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ISOLATION AND CHARACTERIZATION OF CONSTITUENTS OF ESSENTIAL OIL FROM GINGER

Project report submitted to the University of Calicut in partial fulfilment of the requirement for the award of the Degree,

BACHELOR IN CHEMISTRY

By
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(Reg. No. CCAUSCH025)

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THRISSUR, KERALA-680125

APRIL 2023

CANDIDATE'S STATEMENT

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Place: Irinjalakuda
Date: 25/04/2023 MANJIMA M.R.

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ISOLATION AND CHARACTERIZATION OF CONSTITUENTS OF ESSENTIAL OIL FROM GINGER

Project report submitted to the University of Calicut in partial fulfilment of the requirement for the award of the Degree,

BACHELOR IN CHEMISTRY

By
MARIYA GILSON

(Reg. No. CCAUSCH026)

DEPARTMENT OF CHEMISTRY,

CHRIST COLLEGE, IRINJALAKUDA (AUTONOMOUS),

THRISSUR, KERALA-680125

APRIL 2023

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Place: Irinjalakuda
Date: 25/04/2023 MARIYA GILSON

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MARIYA GILSON

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ISOLATION AND CHARACTERIZATION OF CONSTITUENTS OF ESSENTIAL OIL FROM GINGER

Project report submitted to the University of Calicut in partial fulfilment of the requirement for the award of the Degree,

BACHELOR IN CHEMISTRY

By
NAVYA RAJESH

(Reg. No. CCAUSCH027)

DEPARTMENT OF CHEMISTRY,

CHRIST COLLEGE, IRINJALAKUDA (AUTONOMOUS),

THRISSUR, KERALA-680125

APRIL 2023

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Place: Irinjalakuda
Date: 25/04/2023 NAVYA RAJESH

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NAVYA RAJESH

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ONE POT MULTICOMPONENT SYNTHETIC PROTOCOL FOR AMIDO CARBONYL COMPOUNDS

Dissertation submitted to Christ College (Autonomous), Irinjalakuda (University of Calicut) in partial fulfilment of the requirement for the award of Degree of

BACHELOR OF SCIENCE

IN

CHEMISTRY

Submitted by,

NIVED KRISHNA K.P

Reg NoCCAUSCH028

2020-2023

PG AND RESEARCH DEPARTMENT OF CHEMISTRY

CHRIST COLLEGE, IRINJALAKUDA

THRISSUR - 680125

CHRIST
COLLEGE (AUTONOMOUS)
IRINJALAKUDA, KERALA
Reaccredited by NAAC with 'A++' grade

CERTIFICATE

This is to certify that the project work entitled " **ONE POT MULTI COMPONENT SYNTHETIC PROTOCOL FOR AMIDO CARBONYL COMPOUNDS"** is an authentic work done by NIVED KRISHNA K.P (Reg no CCAUSCH028), final semester B.Sc. Chemistry student of this institution under my supervision in partial fulfilment of the requirements for the degree of Bachelor of Science in Chemistry of Christ College (Autonomous), Irinjalakuda (University of Calicut).

Dr. Arun S
Assistant Professor
P.G. And Research Department
Christ College (Autonomous), Irinjalakuda

DECLARATION

I, NIVED KRISHNA K.P (Reg.No.CCAUSCH028) do hereby declare that ,the project work entitle **"ONE POT MULTI COMPONENT SYNTHETIC PROTOCOL FOR AMIDO CARBONYL COMPOUNDS"** submitted to the University of Calicut in Partial Fulfilment of the requirement for the award of the degree of Bachelor of Science was carried under the guidance of Dr.Arun S, Assistant Professor, Department of Chemistry, Christ College, Irinjalakuda and it is a record of original project work carried out by me and it has not previously formed the basis for the award of ,any Degree, Diploma Fellowship or other similar title of recognition by any other university or institutions.

Place: Irinjalakuda NIVED KRISHNA K.P

Date:25th April, 2023

ACKNOWLEDGEMENT

We would like to begin by expressing gratitude to God Almighty for all his blessings.

With great pleasure, we express our sincere gratitude to Dr.Arun S, Associate Professor, Department of Chemistry, Christ College (Autonomous), Irinjalakuda, for his dynamic effort in guiding and instructing us for the completion of this work successfully.

We acknowledge our humble thanks to teachers and non-teaching staffs for their valuable suggestions and help.

Last but not the least, we express thanks to our family, classmates, and friends for being with us, especially when we need them.

NIVED KRISHNA K. P

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Dissertation submitted to Christ College (Autonomous), Irinjalakuda (University of Calicut) in partial fulfilment of the requirement for the award of Degree of

BACHELOR OF SCIENCE

IN

CHEMISTRY

Submitted by,

RIYA LONAPPAN

RegNo.CCAUSCH029

2020-2023

PG AND RESEARCH DEPARTMENT OF CHEMISTRY

CHRIST COLLEGE, IRINJALAKUDA

THRISSUR - 680125

CHRIST
COLLEGE (AUTONOMOUS)
IRINJALAKUDA, KERALA
Reaccredited by NAAC with 'A++' grade

CERTIFICATE

This is to certify that the project work entitled " **ONE POT MULTI COMPONENT SYNTHETIC PROTOCOL FOR AMIDO CARBONYL COMPOUNDS"** is an authentic work done by Riya Lonappan (Reg no CCAUSCH029), final semester B.Sc. Chemistry student of this institution under my supervision in partial fulfilment of the requirements for the degree of Bachelor of Science in Chemistry of Christ College (Autonomous), Irinjalakuda (University of Calicut).

Dr. Arun S
Assistant Professor
P.G. And Research Department
Christ College (Autonomous), Irinjalakuda

DECLARATION

I, Riya Lonappan (Reg.No.CCAUSCH029) do hereby declare that ,the project work entitle **"ONE POT MULTI COMPONENT SYNTHETIC PROTOCOL FOR AMIDO CARBONYL COMPOUNDS"** submitted to the University of Calicut in Partial Fulfilment of the requirement for the award of the degree of Bachelor of Science was carried under the guidance of Dr. Arun S, Assistant Professor, Department of Chemistry, Christ College, Irinjalakuda and it is a record of original project work carried out by me and it has not previously formed the basis for the award of, any Degree, Diploma Fellowship or other similar title of recognition by any other university or institutions.

Place: Irinjalakuda Riya Lonappan

Date:25th April, 2023

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Riya Lonappan

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Dissertation submitted to Christ College (Autonomous), Irinjalakuda (University of Calicut) in partial fulfilment of the requirement for the award of Degree of

BACHELOR OF SCIENCE

IN

CHEMISTRY

Submitted by,

RIYA ROSE THATTIL

RegNo.CCAUSCH031

2020-2023

PG AND RESEARCH DEPARTMENT OF CHEMISTRY

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IRINJALAKUDA, KERALA
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Dr. Arun S
Assistant Professor
P.G. And Research Department
Christ College (Autonomous), Irinjalakuda

DECLARATION

I, Riya Rose Thattil (Reg.No.CCAUSCH031) do hereby declare that ,the project work entitle **"ONE POT MULTI COMPONENT SYNTHETIC PROTOCOL FOR AMIDO CARBONYL COMPOUNDS"** submitted to the University of Calicut in Partial Fulfilment of the requirement for the award of the degree of Bachelor of Science was carried under the guidance of Dr. Arun S, Assistant Professor, Department of Chemistry, Christ College, Irinjalakuda and it is a record of original project work carried out by me and it has not previously formed the basis for the award of, any Degree, Diploma Fellowship or other similar title of recognition by any other university or institutions.

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BACHELOR OF SCIENCE

IN

CHEMISTRY

Submitted by,

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CHRIST
COLLEGE (AUTONOMOUS)
IRINJALAKUDA, KERALA
Reaccredited by NAAC with 'A++' grade

CERTIFICATE

This is to certify that the project work entitled " **ONE POT MULTI COMPONENT SYNTHETIC PROTOCOL FOR AMIDO CARBONYL COMPOUNDS"** is an authentic work done by Sanjay NT (Reg no CCAUSCH031), final semester B.Sc. Chemistry student of this institution under my supervision in partial fulfilment of the requirements for the degree of Bachelor of Science in Chemistry of Christ College (Autonomous), Irinjalakuda (University of Calicut).

Dr. Arun S
Assistant Professor
P.G. And Research Department
Christ College (Autonomous), Irinjalakuda

DECLARATION

I, SANJAY N T(Reg.No.CCAUSCH031) do hereby declare that ,the project work entitle **"ONE POT MULTI COMPONENT SYNTHETIC PROTOCOL FOR AMIDO CARBONYL COMPOUNDS"** submitted to the University of Calicut in Partial Fulfilment of the requirement for the award of the degree of Bachelor of Science was carried under the guidance of Dr.Arun S, Assistant Professor, Department of Chemistry, Christ College, Irinjalakuda and it is a record of original project work carried out by me and it has not previously formed the basis for the award of ,any Degree, Diploma Fellowship or other similar title of recognition by any other university or institutions.

Place: Irinjalakuda SANJAY N T

Date:25th April, 2023

ACKNOWLEDGEMENT

We would like to begin by expressing gratitude to God Almighty for all his blessings.

With great pleasure, we express our sincere gratitude to Dr.Arun S, Associate Professor, Department of Chemistry, Christ College (Autonomous), Irinjalakuda, for his dynamic effort in guiding and instructing us for the completion of this work successfully.

We acknowledge our humble thanks to teachers and non-teaching staffs for their valuable suggestions and help.

Last but not the least, we express thanks to our family, classmates, and friends for being with us, especially when we need them.

SANJAY N T

CONTENTS

ONE POT MULTICOMPONENT SYNTHETIC PROTOCOL FOR AMIDO CARBONYL COMPOUNDS

Dissertation submitted to Christ College (Autonomous), Irinjalakuda (University of Calicut) in partial fulfilment of the requirement for the award of Degree of

BACHELOR OF SCIENCE

IN

CHEMISTRY

Submitted by,

SNEHA ANILKUMAR

RegNo.CCAUSCH032

2020-2023

PG AND RESEARCH DEPARTMENT OF CHEMISTRY

CHRIST COLLEGE, IRINJALAKUDA

THRISSUR - 680125

CHRIST
COLLEGE (AUTONOMOUS)
IRINJALAKUDA, KERALA
Reaccredited by NAAC with 'A++' grade

CERTIFICATE

This is to certify that the project work entitled " **ONE POT MULTI COMPONENT SYNTHETIC PROTOCOL FOR AMIDO CARBONYL COMPOUNDS"** is an authentic work done by Sneha Anilkumar (Reg no CCAUSCH032), final semester B.Sc. Chemistry student of this institution under my supervision in partial fulfilment of the requirements for the degree of Bachelor of Science in Chemistry of Christ College (Autonomous), Irinjalakuda (University of Calicut).

Dr. Arun S
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Christ College (Autonomous), Irinjalakuda

DECLARATION

I, Sneha Anilkumar (Reg.No.CCAUSCH032) do hereby declare that ,the project work entitle **"ONE POT MULTI COMPONENT SYNTHETIC PROTOCOL FOR AMIDO CARBONYL COMPOUNDS"** submitted to the University of Calicut in Partial Fulfilment of the requirement for the award of the degree of Bachelor of Science was carried under the guidance of Dr. Arun S, Assistant Professor, Department of Chemistry, Christ College, Irinjalakuda and it is a record of original project work carried out by me and it has not previously formed the basis for the award of, any Degree, Diploma Fellowship or other similar title of recognition by any other university or institutions.

Place: Irinjalakuda Sneha Anilkumar

Date:25th April, 2023

ACKNOWLEDGEMENT

We would like to begin by expressing gratitude to God Almighty for all his blessings.

With great pleasure, we express our sincere gratitude to Dr. Arun S, Associate Professor, Department of Chemistry, Christ College (Autonomous), Irinjalakuda, for his dynamic effort in guiding and instructing us for the completion of this work successfully.

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Sneha Anilkumar

CONTENTS

DETERMINATION OF OXALIC ACID CONTENT IN BILIMBI FRUIT

Project work

Submitted to Christ College (Autonomous), Irinjalakuda

(University of Calicut) in partial fulfilment of the

requirements for the award of Degree of

BACHELOR OF SCIENCE IN CHEMISTRY

Submitted by

AKSHITHA K.J

Reg.no: CCAUSCH039

RESEARCH AND POSTGRAGUATE

DEPARTMENT OF CHEMISTRY

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IRINJALAKUDA

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This is to certify that the project work entitled "Determination of free oxalic acid content in Bilimbi fruit" is an authentic work done by Akshitha K.J (Reg.no:CCAUSCH039), final semester B.Sc. Chemistry student of this institution under my supervision in partial fulfilment of the requirements for the degree of Bachelor of Science in Chemistry of Christ College (Autonomous), Irinjalakuda (University of Calicut).

Dr. Jibin A K
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Research and Postgraduate
Department Christ College
(Autonomous), Irinjalakuda

Place: Irinjalakuda
Date:27 April 2023

DECLARATION

I Hereby declare that the project work entitled "Determination of free oxalic acid content in Bilimbi fruit" is a work done by me under the guidance of Jibin A. K, Associate Professor of Chemistry, Christ College (Autonomous), Irinjalakuda and has not been included in any other thesis submitted by me for the award of any other degree.

Akshitha K.J

Reg.no: CCAUSCH039

Final Semester B.Sc. Chemistry Student

Christ College (Autonomous), Irinjalakuda

ACKNOWLEDGEMENT

I would like to begin by expressing gratitude to God Almighty for all his blessings.

With great pleasure, I express my sincere gratitude to Dr. Jibin A.K, Assistant Professor, Department of Chemistry, Christ College (Autonomous), Irinjalakuda, for his dynamic effort in guiding and instructing me for the completion of this work successfully.

I acknowledge my humble thanks to teachers and non-teaching staffs for their valuable suggestions and help.

Last but not the least, I express thanks to my family, classmates, and friends for being with me, especially when I need them.

Akshitha K.J

Reg.No: CCAUSCH039

Final Semester B.Sc. Chemistry Student

Christ College (Autonomous), Irinjalakuda.

ABSTRACT

Bilimbi, being a fruit containing high oxalic acid content in it, is taken for investigation. This work focuses on two age groups of bilimbi, ripened and half ripened is observed to have significant difference in its oxalic acid content**.**

CONTENTS

IN SILICO STUDIES ON INHIBITION EFFICENCY OF SOME NATURALLY OCCURRING FLAVONOIDS AGAINST SARS COV-2 RECEPTORS

Dissertation submitted to the Christ College (Autonomous) in partial fulfilment of the requirement for the Degree of

BACHELOR OF SCIENCE

IN

CHEMISTRY

Submitted by

SREELAKSHMI K A

Reg. No: CCAUSCH033

2020-2023

P.G AND RESEARCH DEPARTMENT OF CHEMISTRY

CHRIST COLLEGE, IRINJALAKUDA

THRISSUR-680125

DECLARATION

I, SREELAKSHMI K A (Reg.No.CCAUSCH033) do hereby declare that, this dissertation work entitled "**IN SILICO STUDIES ON INHIBITION EFFICENCY OF SOME NATURALLY OCCURRING FLAVONOIDS AGAINST SARS COV-2 RECEPTORS" s**ubmitted to the University of Calicut in Partial Fulfilment of the requirement for the award of degree of Bachelor of Science was carried under the guidance of Dr.Tom Cherian, Assistant professor, Department of Chemistry, Christ College, Irinjalakuda and it is a record of original project work carried out by me and it has not previously formed the basis for the award of, any degree, Diploma fellowship or other similar title of recognition by any other university or institutions.

Place: Irinjalakuda, SREELAKSHMI K A

Date: 22th April 2023.

CHRIST COLLEGE (Autonomous), IRINJALAKUDA.
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Ref. CC/CHEM/TM/2022-23/02
Date: 22th April 2023

Dr. Tom Cherian
Asst. Professor in Chemistry

CERTIFICATE

This is to certify that SREELAKSHMI K A (Reg.No.CCAUSCH033) has carried out a project work entitled **"IN SILICO STUDIES ON INHIBITION EFFICENCY OF SOME NATURALLY OCCURRING FLAVONOIDS AGAINST SARS COV-2 RECEPTORS"** is an authentic record of the research project carried out by my supervision and guidance in the P.G & Research Department of Chemistry, Christ College, Irinjalakuda. It is further certified that this project report has not previously formed the basis for the award of any Degree, Diploma, Fellowship or other similar title of recognition by any other university or Institutions.

Dr. Tom Cherian

ACKNOWLEDGEMENT

I extend my sincere and heartfelt gratitude to my project guide Dr. Tom Cherian, Department of chemistry, Christ College, Irinjalakuda for his valuable and inspiring guidance, critical assessment and constant encouragement at all stages of this project. I am greatly indebted to him for the completion of this work in the specified period.

I express my sincere thanks to Dr. V T Joy, Head, PG Department of Chemistry, for granting permission to carrying my project. I would like to express my gratitude to all the faculty members in the Department of Chemistry for their inspiration and guidance to complete this work.

I wish to acknowledge my gratitude to Rev. Dr. Jolly Andrews, C.M.I, Principal of Christ College, Irinjalakuda and Library staff of the Christ College for providing the timely help and necessary facilities.

I cheerfully express my profound thanks to all my classmates for their support and co-operation.

Above all I humbly thank God Almighty, whose sustaining grace has been sufficient for me to complete this endeavour.

SREELAKSHMI K A

CONTENTS

IN SILICO STUDIES ON INHIBITION EFFICENCY OF SOME NATURALLY OCCURRING FLAVONOIDS AGAINST SARS COV-2 RECEPTORS

1. INTRODUCTION

1.1 COVID-19

Coronavirus disease 2019(COVID-19) is defined as an illness caused by a novel coronavirus now called Severe Acute Respiratory Syndrome Corona Virus 2 (SARS-CoV-2). It was first identified amid an outbreak of respiratory illness cases in Wuhan city, Hubei province, China in December 31, 2019. On January 30,2020, the WHO declared the COVID-19 outbreak a global health emergency and on March 11, 2020, the WHO declared it a global pandemic. Illness caused by SARSCoV-2 was recently termed COVID-19 by the WHO, the new acronym derived from “coronavirus disease 2019”. Coronaviruses are a large family of zootic viruses that cause illness ranging from the common cold to severe respiratory diseases. Zootic means the viruses are able to be transmitted from animals to humans. There are several corona viruses known to be circulating in different animal populations that have not yet infected humans. COVID-19 is the most recent to make the jump to human infection. Common signs of COVD-19 infection are similar to the common cold and include respiratory symptoms such as dry cough, fever, shortness of breath, and breathing difficulties. In more severe cases, infection can cause pneumonia, severe acute respiratory syndrome, kidney failure and death. COVID-19 virus is primarily transmitted between people through respiratory droplets and contact routes. Droplet transmission occurs when a person is in close contact with someone who has respiratory symptoms (e.g., coughing or sneezing). Transmission may also occur through fomites in the immediate environment around the infected person. Therefore, spread of the virus can occur by direct contact with infected people and indirect contact with surfaces in the immediate environment or with objects used on the infected person. According to current data, time from exposure to onset of symptoms is usually between two and fourteen days, with an average of five days

As on 21st September 2020; COVID-19 (novel RNA virus) has infected >31 million individuals and caused approximately 1 million global deaths [1].

The novel human RNA virus is subjected to the severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) which primarily gains entrance to cells via binding of SARS-CoV-2 Spike glycoprotein to angiotensin converting enzyme 2 (ACE-2) and subsequent endocytosis [2]-[4]. Current news has identified extra entry points, with neuropilin-1 (NRP-1) [5], [6]. Last two decades, the increasing resistances of microorganisms toward antimicrobial agents become severe health trouble so there is a need for a secure, high therapeutic and novel antimicrobial world [7].

1.2 CORONAVIRAL GENOME STRUCTURE

Coronavirus [8] belong to the subfamily Coronavirinae in the family of Coronaviridae of the order Nidovirales, and this subfamily includes four genera: Alphacoronavirus, Betacoronavirus, Gammacoronavirus, and Deltacornavirus. SARS-CoV-2 particles are spherical and has proteins called spikes. These viruses are enveloped particles and its genetic material is positive single stranded RNA. The SARS-CoV-2 virion has a diameter of approximately 1250nm, and its genome ranges from 26 to 32 kilobases. These viruses have 5 structural proteins. They are S protein(Spike), N(nuucleocapsid) protein, E(Envelope) protein, M(Membrane) protein and HE (Hemaglutiresterase) protein. S proteins together with HE protein assist in viral entry to the human cell. S protein attaches to the receptor protein ACE2(Angiotensin Converting Enzyme 2). This S protein give the virus crown like appearance. N protein is a ribonucleoprotein which forms a complex with the RNA to assist in viral assembly. The E protein forms the viral envelope. They are of 2 types: E1 and E2. The E1 is a transmembrane protein matrix and the E2 is a peplogenic glycoprotein. The M protein forms the viral envelope. Hemaglutin is a peplomer with a role in hemaglutination

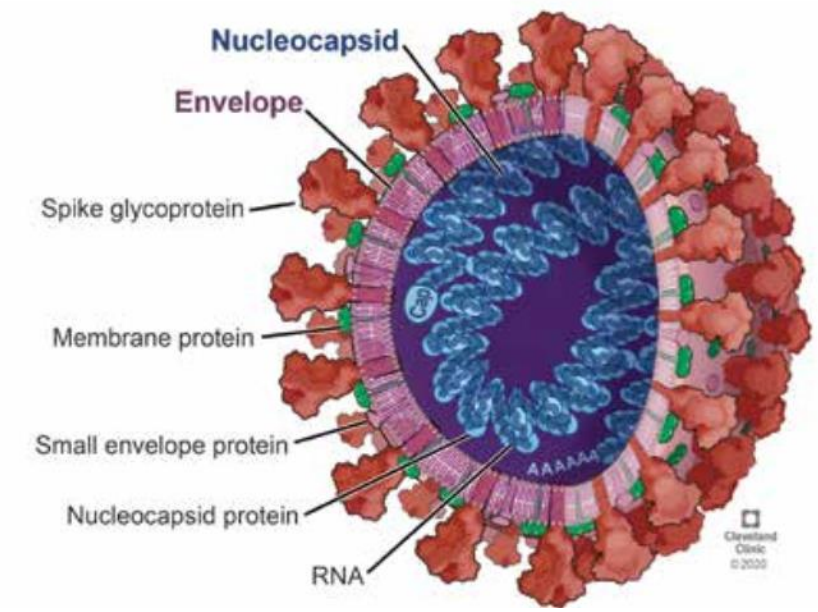


Figure 1: Structure of Corona Virus

1.3 REPLICATION OF CORONAVIRUS

Infection begins when the viral spike protein attaches to its complementary host cell receptor [9]. After attachment, a protease of the host cell cleaves and activates the receptor-attached spike protein. So far, it is not clear whether the virus get into the host cell by fusion of viral and cell membrane or by receptor mediated endocytosis ((in that the virus is incorporated via endosome, which is then acidified by proton pumps). Since coronaviruses have a single positive stranded RNA genome, they can directly produce their protein and new genomes in the cytoplasm. At first, the virus synthesize its RNA polymerase that only recognizes and produces viral RNAs. This enzyme synthesize the minus strand using the positive strand as template. Then the negative strand serves as template to transcribe smaller genomic positive RNAs which are used to synthesize all other proteins. Also, the negative strand serves for replication of new positive stranded RNA genomes. The protein N binds genomic RNA and the protein M is integrated into the membrane of endoplasmic reticulum (ER) like the envelope proteins S and HE. After binding, assembled nucleocapsids with helical twisted RNA bind into the ER lumen and encased with its membrane. These viral progeny are finally transported by the golgi vesicles to the cell membrane and are

exocytosed into the extracellular space. Once released the viruses can infect other host cells.

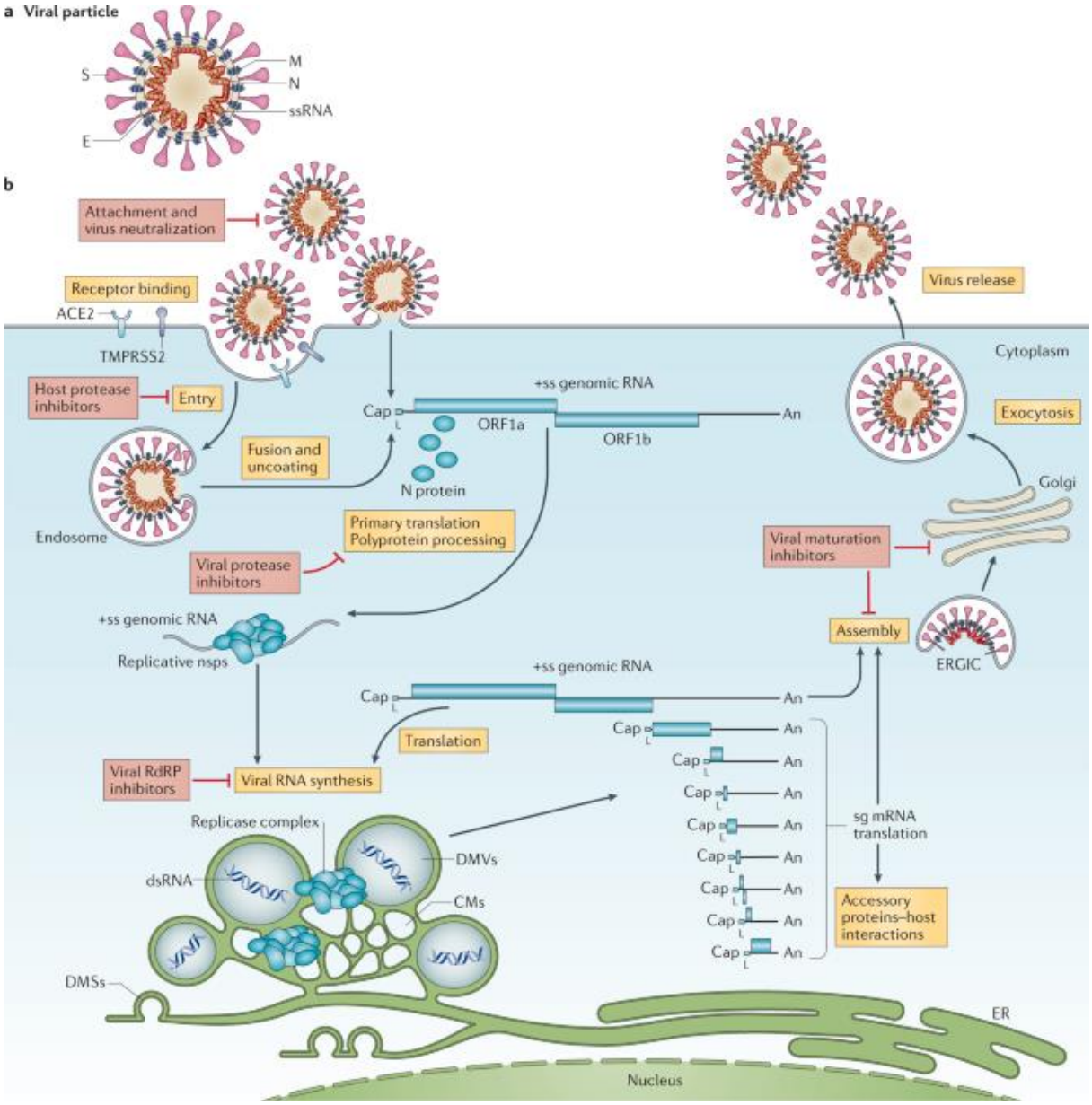


Fig.: Overview of COVID-19, SARS-CoV-2 replication [10]

1.4 RECEPTORS INVOLVED IN VIRUS RNA REPLICATION

There are several functional coronavirus proteins involved in transcription, translation, synthesis, processing and modification of RNA, virus replication and infection [11]. Among these, 3CLpro, PLpro, RdRp and helicase are the most important targets for the development of inhibitors. PLpro is responsible for cleaving the N-terminus of the replicase polyprotein to release Nsp1, Nsp2 and Nsp3, which are essential for viral replication. PLpro is the

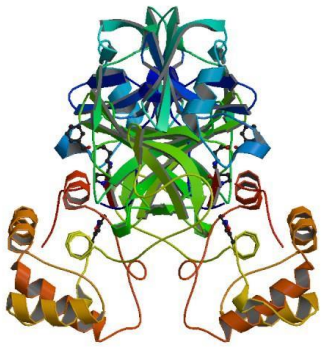
popular target for the inhibitors. 3CLpro (chymotrypsin-like protease), also known as Nsp5, is first automatically cleaved from polyproteins to produce mature enzymes and then further cleaves Nsps downstream at 11 sites to release Nsp4-Nsp16. 3CLpro directly mediates the maturation of the Nsps, essential in the life cycle of the virus. RNA dependent RNA polymerase or RdRp is responsible for polymerisation of viral RNA

1.5 CRYSTALLOGRAPHIC STRUCTURES OF PROTEINS

The crystallographic structures of the target proteins were obtained using the Protein Data Bank (PDB). The two characterization methods are Electron Microscopy and X-ray diffraction. [https://www.rcsb.org/]

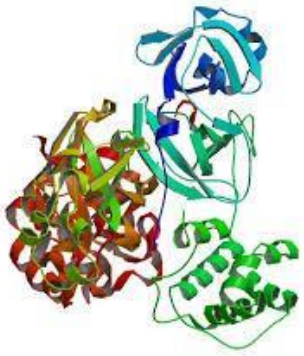
SARS Cov-2-M^{pro}

The crystallographic structure of main protease SARSCoV-2 used in this work has a high resolution of 2.16Å, containing a total of 306 residues and approximately 31.4kDa of molecular mass.

	Crystal structure of SARS coronavirus main protease with PDB ID:6LU7

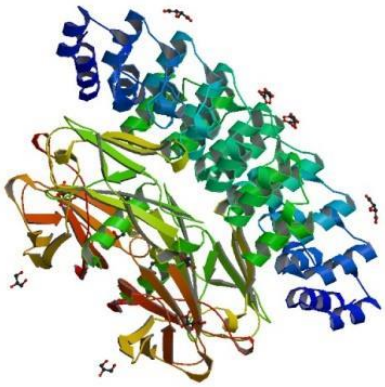
SARS CoV 3CL^{pro}

The protein SARS-CoV3CL^{pro} has a resolution of 2.50Å with a total of 603 residues and approximately 62.0kDa of molecular mass

	Crystal structure of SARS corona virus main protease with PDB ID:1UK4

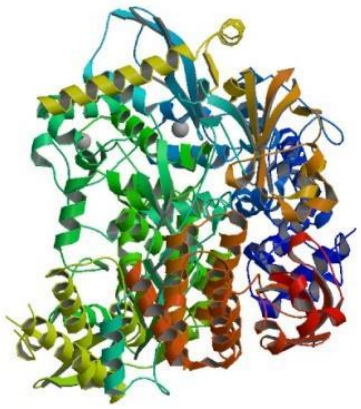
ACE-2 receptor with spike receptor domain of viral protein

The complex of SARS-CoV-2 spike with ACE2 receptor has a resolution of 2.45Å with a total of 791 residues and a molecular mass near of 84.8kDa

	Crystal structure of ACE2 receptor with PDB ID: 6M0J

NSP12 RNA POLYMERASE

This protein is also called RNA dependent RNA polymerase (RdRp). The complex of SARS-Coronavirus NSP12 and NSP7, NSP8 co-factors used an Electron Microscopy to determine the structure. It has a resolution of 3.10Å and a total of 1435 amino acid residues. It's molecular mass is near 114.54kDa

	SARS-Coronavirus NSP12 with PDB ID: 6NUR

1.6 DRUGS USED IN COVID 19

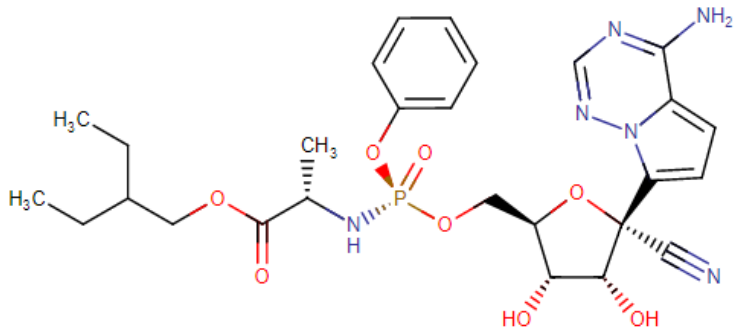
REMDESIVIR

Remdesivir is a nucleoside analog used to treat RNA virus infections including COVID-19. Severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) is the causative agent of coronavirus disease 2019 (COVID-19), which is a respiratory disease that is capable of progressing to viral pneumonia and acute respiratory distress syndrome (ARDS); COVID-19 can be fatal. Like other RNA viruses, SARS-CoV-2 depends on an RNA-dependent RNA polymerase (RdRp) enzyme complex for genomic replication, which can be inhibited by a class of drugs known as nucleoside analogues. [12]

Remdesivir (GS-5734) is an adenosine triphosphate analogue first described in the literature in 2016 as a potential treatment for Ebola [13,14]. Broad antiviral activity of remdesivir is suggested by its mechanism of action, [12]and to date, it has demonstrated *in vitro* activity against the *Arenaviridae*, *Flaviviridae*, *Filoviridae*, *Paramyxoviridae*, *Pneumoviridae*, and Coronaviridae viral families. [14]. Remdesivir activity against the *Coronaviridae* family was first demonstrated in 2017, [15]. leading to considerable interest in remdesivir as a possible treatment for COVID-19.[16,17]. Remdesivir was confirmed as a non-obligate chain terminator of RdRp from

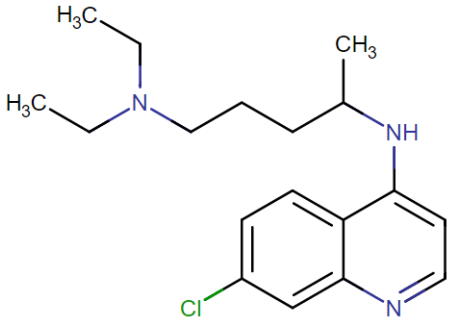
SARS-CoV-2 and the related SARS-CoV and MERS-CoV, [12], and has been investigated in multiple COVID-19 clinical trials.

Based on aggregate data, remdesivir was granted an FDA Emergency Use Authorization (EUA) on May 1st, 2020. The FDA subsequently granted full approval for remdesivir as a COVID-19 treatment on October 22, 2020, while simultaneously updating the EUA to cover those patients not included under the approved indication. Remdesivir is currently marketed under the trademark name VEKLURY by Gilead Sciences Inc. Remdesivir in combination with baricitinib for the treatment of COVID-19, was granted an FDA Emergency Use Authorization on 19 Novermber 2020.

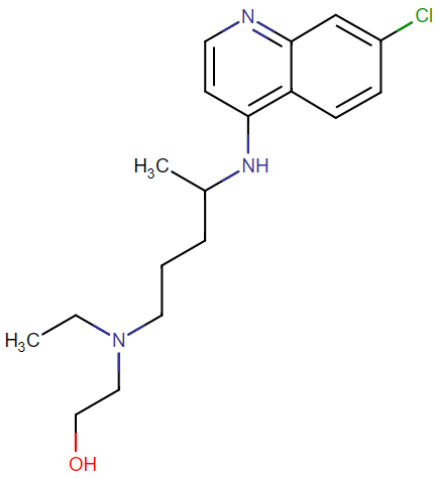


CHLOROQUINE

Chloroquine is an antimalarial drug used to treat susceptible infections with P. vivax, P. malariae, P. ovale, and P. falciparum. It is also used for second line treatment for rheumatoid arthritis. Chloroquine is an aminoquinolone derivative first developed in the 1940s for the treatment of malaria. It was the drug of choice to treat malaria until the development of newer antimalarials such as pyrimethamine, artemisinin, and mefloquine. Chloroquine and its derivative hydroxychloroquine have since been repurposed for the treatment of a number of other conditions including HIV, systemic lupus erythematosus, and rheumatoid arthritis.[18]. The FDA emergency use authorization for hydroxychloroquine and chloroquine in the treatment of COVID-19 was revoked on 15 June 2020.

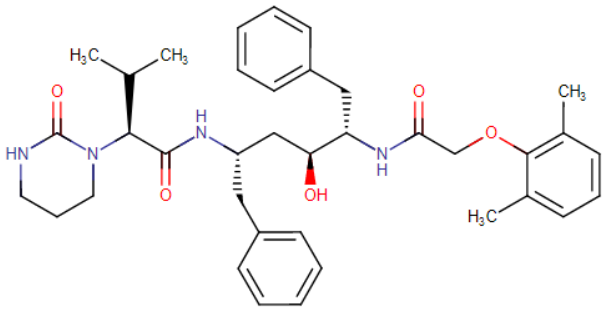


Hydroxychloroquine is an antimalarial medication used to treat uncomplicated cases of malaria and for chemoprophylaxis in specific regions. Also a disease modifying anti-rheumatic drug (DMARD) indicated for treatment of rheumatoid arthritis and lupus erythematosus. Hydroxychloroquine is a racemic mixture consisting of an R and S enantiomer. Hydroxychloroquine is an aminoquinoline like chloroquine. It is a commonly prescribed medication in the treatment of uncomplicated malaria, rheumatoid arthritis, chronic discoid lupus erythematosus, and systemic lupus erythematosus. Hydroxychloroquine is also used for the prophylaxis of malaria in regions where chloroquine resistance is unlikely. It was developed during World War II as a derivative of quinacrine with less severe side effects [19]. Chloroquine and hydroxychloroquine are both being investigated for the treatment of SARS-CoV-2 [20].The FDA emergency use authorization for hydroxychloroquine and chloroquine in the treatment of COVID-19 was revoked on 15 June 2020. A recent study reported a fatality in the group being treated with hydroxychloroquine for COVID-19[21].



KALETRA(LOPINAVIR/RITONAVIR)

Lopinavir is an HIV-1 protease inhibitor used in combination with ritonavir to treat human immunodeficiency virus (HIV) infection. Lopinavir is an antiretroviral protease inhibitor used in combination with other antiretrovirals in the treatment of HIV-1 infection. Lopinavir is marketed and administered exclusively in combination with ritonavir - this combination, first marketed by Abbott under the brand name Kaletra in 2000, is necessary due to lopinavir's poor oral bioavailability and extensive biotransformation. Ritonavir is a potent inhibitor of the enzymes responsible for lopinavir metabolism, and its co-administration "boosts" lopinavir exposure and improves antiviral activity. Like many other protease inhibitors (e.g. saquinavir, nelfinavir), lopinavir is a peptidomimetic molecule - it contains a hydroxyethylene scaffold that mimics the peptide linkage typically targeted by the HIV-1 protease enzyme but which itself cannot be cleaved, thus preventing the activity of the HIV-1 protease [22]. Lopinavir is currently under investigation in combination with ritonavir for the treatment of COVID-19 caused by SARS-CoV-2 [23].



1.7 LITERATURE REVIEW

Nitrogen & sulphur containing heterocyclic [24] compounds have significantly a lot of interest due to the wider application of pharmacological activity. Pyrimidine may perhaps be a basic nucleus in DNA & RNA; it is related with different biological activities like antibacterial [25], antifungal [26]-[29], antibiotics [30], anticancer [31], [32], anti-diabetic [33], anti-tubercular [34], anti-malarial [35], anti-HIV [36], antiviral [37]-[40], antioxidant

[41] and anti-inflammatory [42]. The literature review reveals that mutual pyrimidine and biguanidine derivatives [43-46] are exhibits tremendous biological activities. Moving forward by this study, we synthesized a novel series of pyrimidine derivatives by incorporating the biguanidine moiety with the hope of superior therapeutic agents. The versatility of the infant generation of the novel pyrimidines will constitute a rewarding pharmacophore.

In-silico ADMET [47-49] predictions using ADMETlab2.0 software will further boost our aptitude to guess and representation the most significant pharmacokinetic, metabolic and toxicity endpoints, so accelerating the pills discovery route.

Flavonoids are an important kind of natural products. Flavonoids are a diverse group of phytonutrients (plant chemicals) found in almost all fruits and vegetables.

Along with carotenoids, they are responsible for the vivid colors in fruits and vegetables. Flavonoids are the largest group of phytonutrients, with more than 6,000 types. In particular, they belong to a type of plant secondary metabolites with a polyphenolic structure widely found in fruits and vegetables. They have miscellaneous reciprocal biochemical and antioxidant effects associated with various diseases such as cancer, Alzheimer's disease and atherosclerosis. It is due to antioxidants, anti-inflammatory, anti-mutagens and anti-cancer-causing properties combined with the ability to control major cell enzyme functions. Intriguingly, some flavonoids also have antiviral activity. There are several significant groups of flavonoids, including anthocyanidins, flavanols, flavones, flavononols, flavonones, biflavanoids, isoflavones etc. Each of these subgroups and each type of flavonoid carries its own distinct set of actions, benefits and originating foods Currently, there is no appropriate treatment for SARS-CoV-2 or vaccine alive to care for humans from such infections. It is extremely urgent to build up numerous therapeutic agents

for SARS-CoV-2 virus because of its high infection, morbidity and its ability to cause epidemics universally. In addition, the primary drug discovery pipeline we introduced to the molecular docking studies against seven important target proteins like a spike, SARS Cov-2-M^{pro}, SARS CoV $3CL^{pro}$ and ACE-2 protein, can be potential druggable targets. From the literature studies it is clear that flavonoids having antiviral activity, in the present study we were selected three naturally occurring flavanols such as: Quercetin, Fisetin and Rutin (found in Yellow onion, Curly kale, Leek, Cherry, Tomato, Broccoli, Apple, Green and black tea, Black grapes, Blue berry) for docking studies. The docking study compared with currently used human trial drugs such as Hydroxychloroquine, Favipiravi and Lopinavir/ritonavir (http://www.redo- project.org/covid19db/).

2. METHODOLOGY

2.1 **Computer - Assisted Drug Design (CADD)**

Computer-aided drug design uses computational approaches to discover, develop, and analyse drugs and similar biologically active molecules. The objective of drug design is to find a chemical compound that can fit to a specific cavity on a protein target both geometrically and chemically. Binding of ligands to the receptor may include hydrophobic, electrostatic, hydrogen-bonding and vander waals interactions. Depending on the availability of structural information, a structure based approach or a ligand based approach is used.

STRUCTURE BASED APPROACH

In SBDD, structure of the target protein is known and interaction or bio-affinity for all tested compounds is calculated after the process of docking to design a new drug molecule, which shows better interaction with the target protein. In structure-based drug designing, the structural information obtained

from the x-ray crystallographic studies of the biological target made in a solution would be used as an ideal starting point for CAAD. Theoretical and computational techniques are used to mimic the behavior of molecular system and no experimental data is needed to build models of the ligand and receptor using computational methods. After the biological target has been defined, the next step is to determine the proper binding site. Then different compounds from the database is screened for the best fitting to the binding site and then scored regarding its affinity for the site. The compounds with best affinity towards the binding site of the macromolecule are selected. The problem with docking is to design ligands that will interact favorably at the site. The method is less tedious since screening is by docking and the active structures need to be synthesized.

LIGAND BASED APPROACH

In LBDD, 3D structure of the target protein is not known but the knowledge of ligands which binds to the desired target site is known. These ligands can be used to develop a pharmacophore model or molecule which possesses all necessary structural features for bind to a target active site. Generally, ligand-based techniques are pharmacophore-based approach and quantitative-structure activity relationships (QSARs). In LBDD it is assumed that compounds which having similarity in their structure also having the same biological action and interaction with the target protein

2.2 VIRTUAL SCREENING

Virtual screening has been worked as a most convenient tool now a day to find out the most favorable bioactive compounds with the help of information about the protein target or known active ligands. In the recent time virtual screening is known as a mind-blowing alternative of high-throughput screening

mainly in terms of cost effectiveness and probability of finding most appropriate novel hit through filter the large of libraries of compounds

2.3 MOLECULAR DOCKING

The molecular docking approach can be used to model the interaction between a small molecule and a protein at the atomic level, which allow us to characterize the behavior of small molecules in the binding site of target proteins as well as to elucidate fundamental biochemical processes [19]. The docking process involves two basic steps: prediction of the ligand conformation as well as its position and orientation within these sites (usually referred to as *pose*) and assessment of the binding affinity. These two steps are related to sampling methods and scoring schemes, respectively, which will be discussed in the theory section.

Knowing the location of the binding site before docking processes significantly increases the docking efficiency. In many cases, the binding site is indeed known before docking ligands into it. Also, one can obtain information about the sites by comparison of the target protein with a family of proteins sharing a similar function or with proteins co-crystallized with other ligands. In the absence of knowledge about the binding sites, cavity detection programs or online servers, e.g. GRID[20, 21], POCKET [22], SurfNet [23, 24], PASS [25] and MMC [26] can be utilized to identify putative active sites within proteins. Docking without any assumption about the binding site is called blind docking.

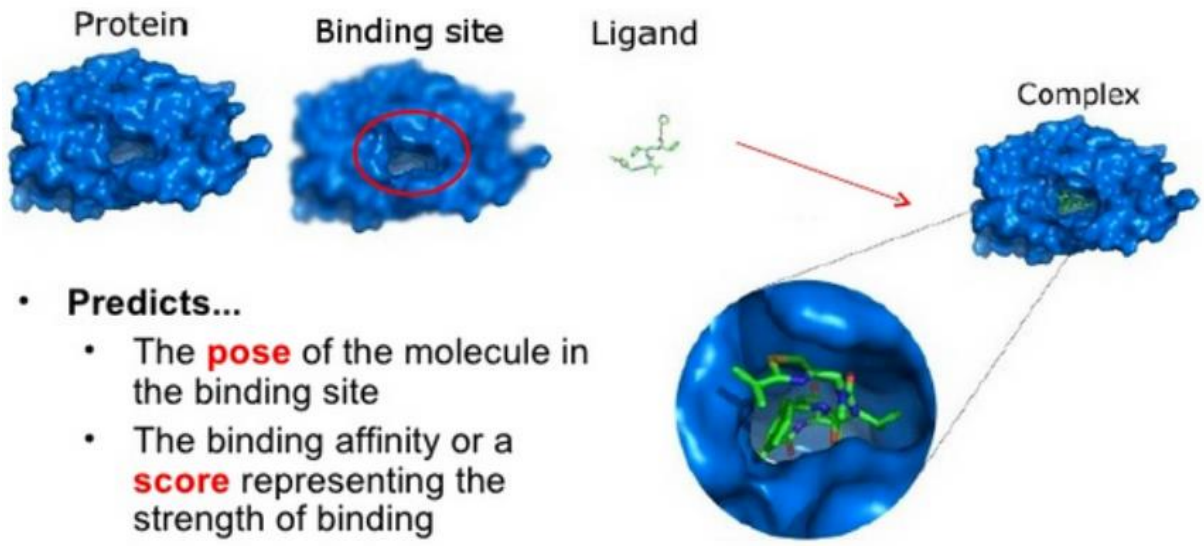
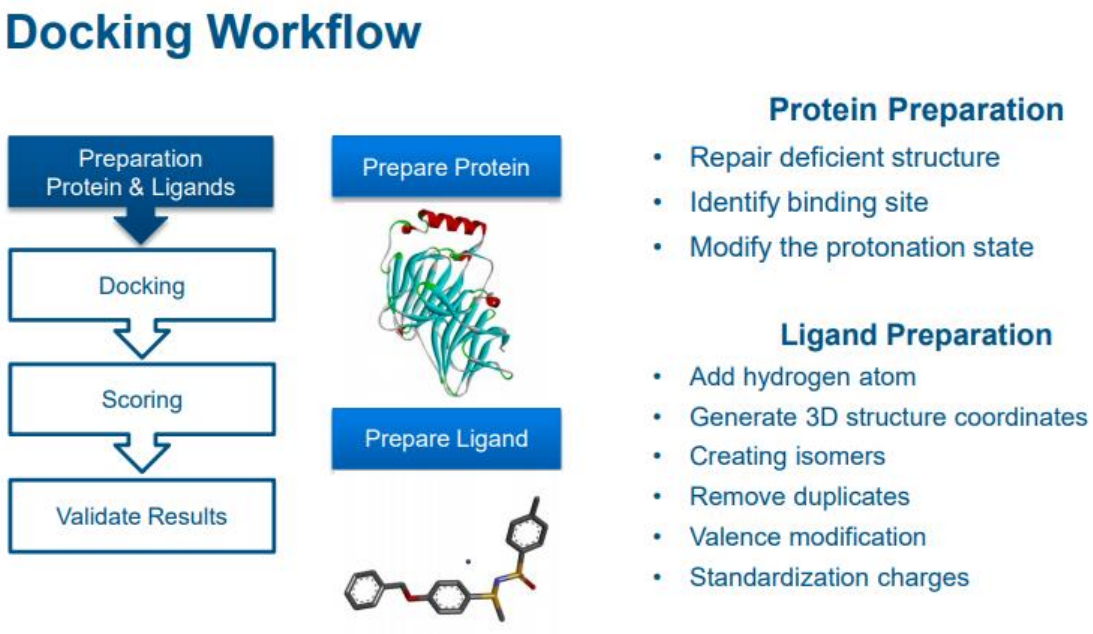


Fig: Ligand Docking- A Graphical Summary



Molecular docking is in-silico method which predicts the placement of small molecules or ligands within the active site of their target protein (receptor). It is mainly used to accurate estimation of most favourable binding modes and bio-affinities of ligands with their receptor, presently it has been broadly applied to virtual screening for the optimization of the lead compounds. Molecular docking methodology comprises mainly three goals which are interconnected to each other like: prediction of binding pose, bio affinity and virtual screening. In

the molecular docking method the basis tools are search algorithm and scoring functions for creating and analysing conformations of the ligand.

BINDING FREE ENERGY ESTIMATION

The binding free energy of the protein–ligand complexes was calculated using MM-PBSA (Molecular Mechanics Poisson-Boltzmann Surface Area), which describes the structural stability, spatial orientation and molecular interactions of ligands in the active site of the protein. The binding free energy abbreviated as DG binding can be defined as

$$\Delta \boldsymbol{G_{Binding}} = < \Delta \boldsymbol{G_{Complex}} > -(< \Delta \boldsymbol{G_{Protein}} > + < \Delta \boldsymbol{G_{Ligand}} >)$$

where $G_{complex}$ represents the total free energy of protein-ligand complex, $G_{protein}$ as the free energy of protein, G_{ligand} used as the free energy of ligand and < > represents the ensemble average.

Neglecting the entropy term (TDS), the binding free energy can be approximately written as

$$\Delta \boldsymbol{G_{Binding}} = \Delta \boldsymbol{E_{MM}} + \Delta \boldsymbol{G_{Solv}}$$

where ΔE_{MM} is the change in the molecular mechanics interaction energy (gas-phase) upon ligand binding calculated as the sum of the changes in the bonded energy, electrostatics and Van der Waals interactions upon ligand binding. ΔG_{solv} is the change in solvation free energy upon ligand binding. Furthermore, ΔG_{solv} can be written as

$$\Delta \boldsymbol{G_{Solv}} = \Delta \boldsymbol{G_{POL}} + \Delta \boldsymbol{G_{NP}}$$

where ΔG_{POL} is the change in the polar part of solvation free energy and ΔG_{NP} is the change in nonpolar part of solvation free energy as a result of ligand binding to the proteins. In this work, Poisson–Boltzmann (PB) method was used for the estimation of the polar part of the solvation free energy

2.4 DIFFERENT DOCKING TOOLS

1-Click Docking (2011) : Docking predicts the binding orientation and affinity of a ligand to target AADS (2011): Automated active site detection, docking, and scoring (AADS)-protocol for proteins with known structures based on Monte Carlo Method. AutoDock (1990): Automated docking of ligand to macromolecule by Lamarckian Genetic Algorithm and Empirical Free Energy Scoring Function. AutoDock Vina (2010): New generation of AutoDock. Beta Dock (2011): Based on Voronoi Diagram. Blaster (2009): Combines ZINC databases with DOCK to find ligand for target protein. BSP-SLIM (2012): A new method for ligand-protein blind docking using low resolution protein structure

2.5 MOLECULAR DOCKING USING CHIMERA AND AUTODOCK VINA SOFTWARE

AutoDock Vina is an open-source program for doing molecular docking. It was designed and implemented by Dr. Oleg Trott in the Molecular Graphics Lab at The Scripps Research Institute. Auto Dock Vina significantly improves the average accuracy of the binding mode predictions. Auto Dock Vina has been tested against a virtual screening and was found to be a strong docking program. For its input and output, Vina uses PDBQT files format used by Auto Dock. PDBQT files can be generated and viewed using MGL Tools.

UCSF Chimera (or simply Chimera) is an extensible program for interactive visualization and analysis of molecular structures and related data, including density maps, supramolecular assemblies, sequence alignments, docking results, trajectories, and conformational ensembles. High-quality images and movies can be created. Chimera includes complete documentation and can be downloaded free of charge for non-commercial use. Chimera is developed by the Resource for Biocomputing, Visualization, and Informatics (RBVI) at the University of California, San Francisco. Development is partially supported by the National Institutes of Health (NIGMS grant P41-GM103311).

2.6 METHODOLOGY OF THE CURRENT PROJECT

The docking procedure was established to study the binding affinity of some flavonoids with major proteins found in SARS-CoV 2 virus. The chemical structures of different flavonoids were obtained from PubChem database. The crystallographic structures of SARS-CoV-2 Mpro (6LU7), SARS-CoV 3CLpro (1UK4), ACE2 receptor (6MOJ) and NSP12RNA Polymerase (6NUR) are obtained from RSCB.PDB database. Then we studied the protein-ligand interactions using docking procedure.

The protein structures were opened in Chimera software. Any ligands or water molecules were removed to get the protein alone and polar hydrogens were added. The file is then saved in c folder with a different file name. Then this file is opened in Chimera and saved in PDB format. The structures of flavonoids are obtained from PubChem database in mol2 or sdf format. The pdb files of proteins were opened in Discovery Studio and find the binding site and grid coordinates. The PDB files of proteins and active compounds were saved in C drive with text config file and vina application. The docking process was done by using Auto Dock Vina. This process was run by using command prompt. Once the process was complete, we get the binding energies of the ligands bound to the receptors as the result. The pose with highest binding energy (best pose) is noted and saved in PDBQT format. Now the result is analysed using Discovery studio. The PDBQT files of both the receptor and the output opened in Discovery studio. Then the different types of interactions were identified.

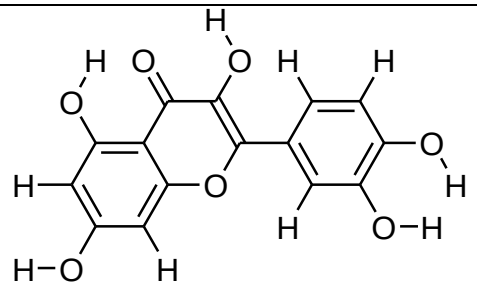
ADMET SCREENING

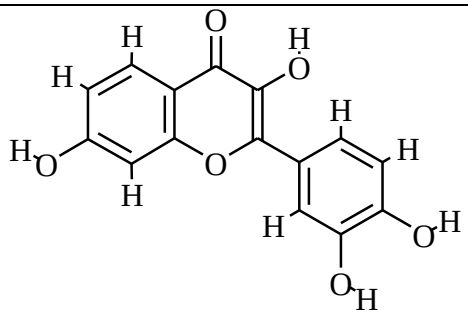
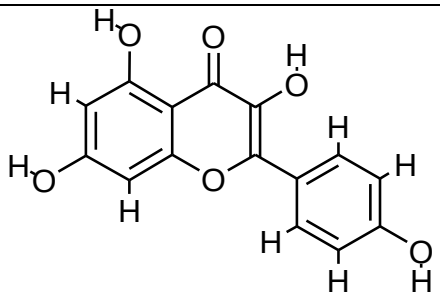
ADMET Predictor is a machine learning software tool that quickly and accurately predicts over 175 properties including solubility, logP, pKa, sites of CYP metabolism, and Ames mutagenicity. Chemical absorption, distribution, metabolism, excretion, and toxicity (ADMET), play key roles in drug discovery and development. In this study, we proposed a scoring function named the ADMET-score to evaluate drug-likeness of a compound.

The Toxicity Forecaster (Tox Cast) project uses quantitative high-efficiency screening to predict the chemical toxicity of several biological pathways that follow the NTP guidelines. One main reason for R&D failures is the efficacy and safety deficiencies which are related largely to absorption, distribution, metabolism and excretion (ADME) properties and various toxicities (T). Therefore, rapid ADMET evaluation is urgently needed to minimize failures in the drug discovery process. Over the past two decades, an in silico absorption, distribution, metabolism, and excretion (ADMET) platform has been created at Bayer Pharma with the goal to generate models for a variety of pharmacokinetic and physicochemical endpoints in early drug discovery.

OPs provide data needed to determine the potential safety or toxicity of a drug. Drug metabolism and interaction data provide researchers with the information they need to determine the likelihood of drug–drug interactions (DDIs). Anticipating drug interactions is essential for safe pharmaceutical development. ADME-Tox properties relate to the absorption, distribution, metabolism, excretion, and toxicity of a drug molecule. Traditionally, these properties were predicted at the end of the drug discovery pipeline; however, with the advancement of in-silico tools such properties can be predicted in the early phase.

SELECTED FLAVANOLS COMPOUNDS FOR STUDIES

A	 2-(3,4-Dihydroxy-phenyl)-3,5,7-trihydroxy-chromen-4-one (Quercetin)

B	 2-(3,4-Dihydroxy-phenyl)-3,7-dihydroxy-chromen-4-one (Fisetin)
C	 3,5,7-Trihydroxy-2-(4-hydroxy-phenyl)-chromen-4-one (Kaempferol)

3. RESULT AND DISCUSSIONS

Web based PASS (Prediction of Activity Spectra for Substances; http://www.way2drug.com/passonline/) [45-47] predication selective results are presented in Table 2. The data indicated that these selected flavonoids [A, B & C] are active against Antiviral (Influenza) and Antiviral (HIV).

Table 2. Predicted biological activities of selected compound using PASS software

Drug	Antiviral (Influenza)		Antiviral (HIV)	
A	0,403	0,046	0,262	0,053
B	0.352	0.087	0,113	0,081
C	0,400	0,047	0,164	0,051

Pa = Probability ‘to be active’; Pi = Probability ‘to be inactive’

3.1 ADMET PREDICTION

In the present study ADMET (absorption, distribution, metabolism, excretion, and toxicity) properties of the SEs was calculated from pkCSM online server

(http://biosig.unimelb.edu.au) [48]. It should be noted that ADMET are the most important properties of pharmacokinetic (PK) profiles. As shown in Table 3, the SEs have good absorption especially human intestinal absorption and comparable to the standard drug fluconazole. All the selected flavanols compounds A, B and C are P-glycoprotein inhibitor. P-glycoprotein inhibition can interrupt the absorption, permeability and retention of the chemical species. Their distribution through blood brain barrier (BBB) and central nervous system (CNS) are almost similar to that of fluconazole. However, these compounds can metabolize easily as they aren't CYP3A4 enzyme substrate. Their excretion through renal system is excellent and better than the fluconazole. They aren't human ether-a-go-go-related gene (hERG) inhibitor, and hence, they can be used as safe drug as hERG inhibitor causes fatal long QT syndrome to human. Their safer use is further supported by their low rat acute toxicity value (expressed as LD50, Table 3). Toxicity calculation has become essential in the drug discovery process because about30% of drug molecules did not clear the clinical trials because of their toxicity. COVID-19 epitomic, in-silico studies also have been used for their process of drug discovery. It was concluded that selected naturally occurring flavonoids [A, B and C] may be a promising hit molecule for the development of novel COVID therapeutics.

Toxicity calculation has become essential in the drug discovery process because about 30% of drug molecules did not clear the clinical trials because of their toxicity. COVID-19 epitomic, in-silico studies also have been used for their process of drug discovery. It was concluded that the naturally occurring flavonoids (A-C) may be a promising hit molecule for the development of novel COVID therapeutics.

Table-3: ADMET properties of the selected compounds using pkCSM server.

Drug	Absorption			Distribution		Metabolism	Excretion	Toxicity	
	C2P	HIA (%)	P-gpI	BBB (permeability)	CNS	CYP3A4 substrate	Total clearance	hERG (Inhibitor)	LD_{50} (Rat)
A	1.021	75.34	Yes	-1.377	-3.47	No	0.663	No	1.944
B	0.716	85.46	Yes	-1.114	-1.11	No	0.557	No	2.111
C	1.031	75.48	Yes	-1.223	-2.37	No	0.655	No	2.301

C2P = Caco-2 permeability (log Papp in 10-6 cm/s, >0.90 indicates high permeability); HIA = Human intestinal absorption (% absorbed, >30% is better absorbed); P-gpI = P-glycoprotein inhibitor; BBB (blood brain barrier) is expressed in logBB (logBB >-1.0 is moderately cross blood brain barrier); CNS is expressed as logPS (logPS>-2.0 can easily penetrate the CNS); Total clearance is expressed in log mL/min/kg; Toxicity is calculated in oral rat acute toxicity (mol/kg); FCZ = fluconazole.

Considering the medicinal importance of the flavonoids derivatives, additional drug likeness properties are mentioned in Table 4 as calculated from the Swiss ADME [49]. Swiss ADME calculation indicated that all the SEs have good hydrogen bonds donor or acceptor

Table 4. Calculation drug likeliness using Swiss ADME programme.

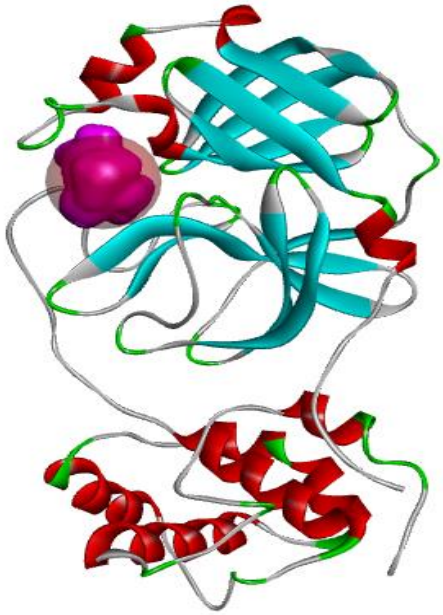
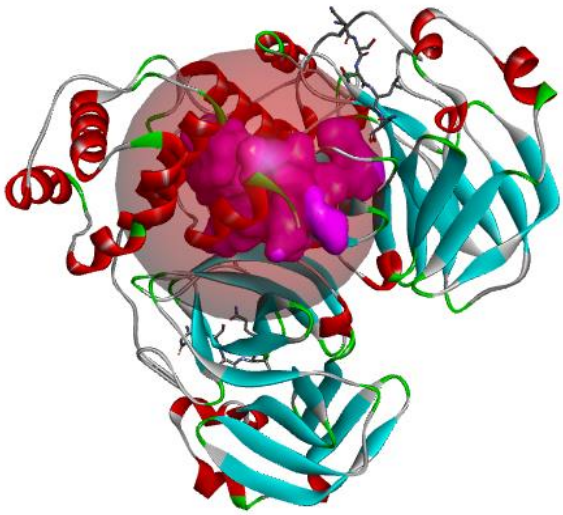
Drug	HBA	HBD	TPSA Å²	Rotatable bonds	log p	GI absorption	PAINS alerts
A	7	5	131.36	1	2.155	High	0
B	6	4	111.13	1	2.28	High	0
C	6	4	111.13	1	2.28	High	0

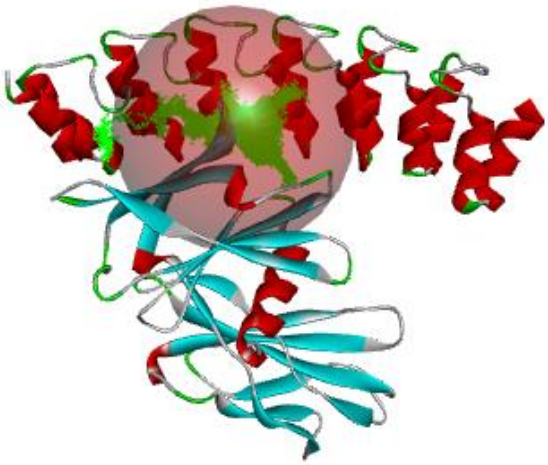
*HBA = Hydrogen bond acceptor, HBD = Hydrogen bond donor, TPSA = Topological polar surface area, GI = Gastrointestinal; PAINS = Pan-assay interference compounds

Topological polar surface area (TPSA) data showed the good agreement with the acceptable values (below 86 Å2) where the TPSA value should be less than 140 Å2 (Fig. 4). With the increase of the chain length of the acyl group(s) their water solubility decreased. Gastrointestinal absorption of A, B and C are high. More importantly, none of the SEs violates Pan-assay interference compounds (PAINS) whereas positive PAINS value indicates false results in high-through put screens with numerous biological targets. Overall, drug likeness scores of selected flavanols compounds A, B and C using Molsoft's chemical fingerprints are found to be moderate.

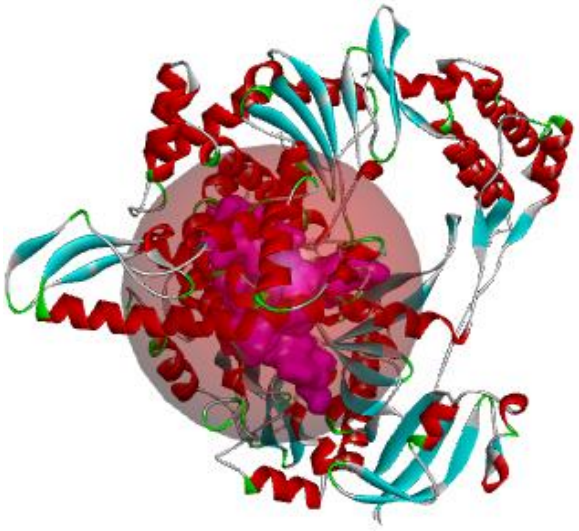
3.2 BINDING SITE PREDICTION USING BIOVIA DISCOVERY STUDIO VISUALIZER

Potential binding site of protein is determined using BIOVIA visualizer software.

6LU7	**1UK4**
	
X=-13.67, Y=14.92, Z=73.81	**X=66.43, Y=-22.31, Z=15.68**
6MOJ	**6NUR**



X=-44.13, Y=-31.84, Z=22.36



X=152.93, Y=159.78, Z=150.28

3.3 MOLECULAR DOCKING STUDIES

Table 5: Docking Results of the Designed Compounds (A-C) Towards COVID-19 Proteins.

Ligand	Binding Energy 6LU7 (k.cal/mol)	Binding Energy 1UK4 (k.cal/mol)	Binding Energy 6M0J (k.cal/mol)	Binding Energy 6NUR (k.cal/mol)
A	-7.2	-8.9	-8.4	-8.6
B	-7.4	-8.9	-8.5	-8.2
C	-7.7	-8.5	-7.9	-8.3
Hydroxychloroquine	-4.9	-5.7	-4.5	-5.1
Favipiravir	-5.8	-6.0	-5.5	-6.6
Lopinavir	-8.1	-7.2	-7.0	-8.

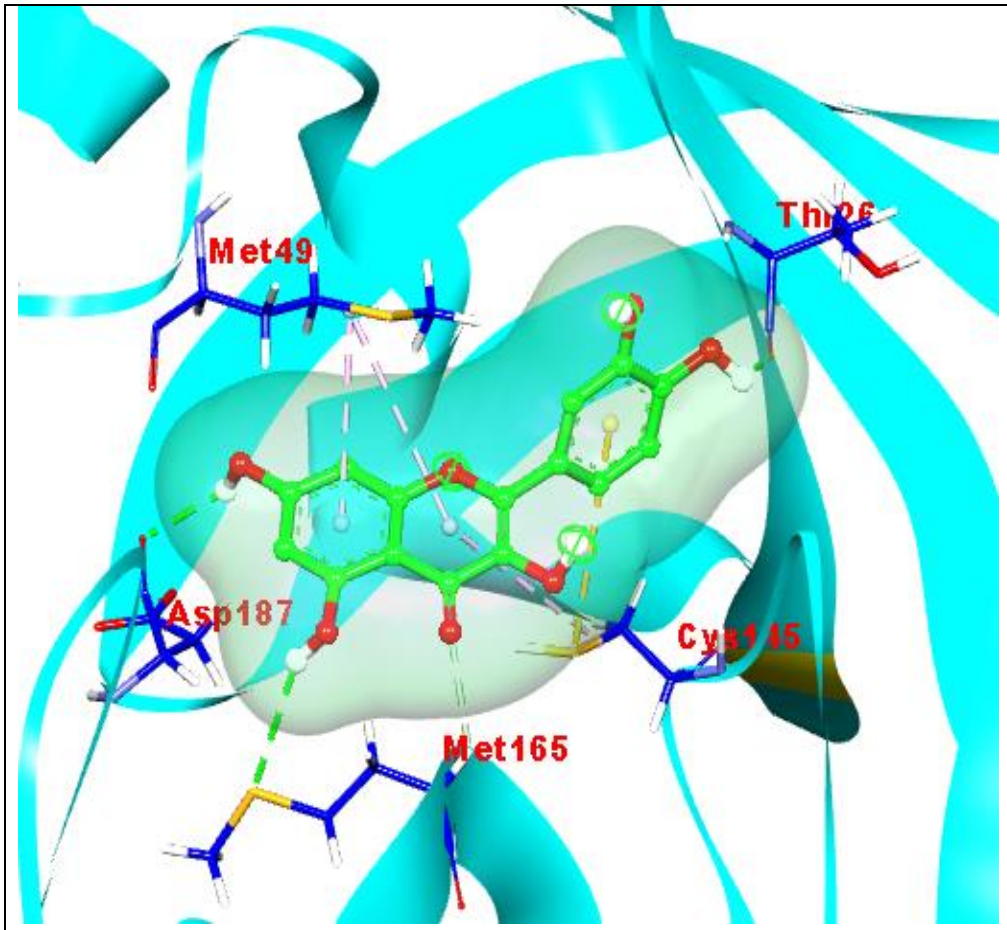
Auto Dock Vina 1.1.2 (for window) is one of the freely existing software, crucially used to introductory molecular docking. The software offers multi-core capability, high performance, enhanced accuracy and ease of use. The target COVID-19 3D protein structures (6LU7, 1UK4, 6MOJ and 6NUR) were downloaded from protein data bank (PDB) and then

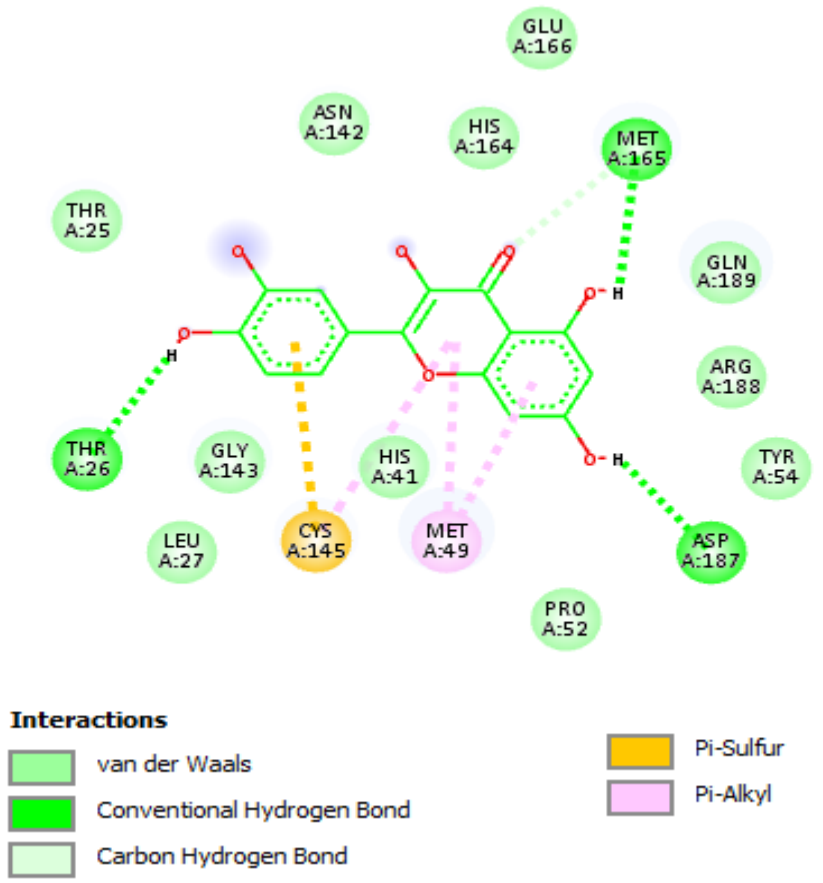
converted into pdbqt format. The selected ligands (7A-7C) were subjected to a molecular docking study against four important COVID-19 viral proteins. Protein and ligands preparations and their docking process are followed regular protocol and the discovery studio 4.5 (viewer) is used for the imaging process. Among the sequence of compounds, 7A ligand showing binding energy against four [6LU7, 1UK4, 6MOJ and 6NUR] proteins with binding energies -7.2 kcal/mol, -8.9 kcal/mol, -8.4 kcal/mol and -8.6 kcal/mol respectively. 7B ligand showing binding energy against four [6LU7, 1UK4, 6MOJ and 6NUR] proteins with binding energies -7.4 kcal/mol, -8.9 kcal/mol, -8.5 kcal/mol and -8.2 kcal/mol respectively. 7C ligand showing binding energy against four [6LU7, 1UK4, 6MOJ and 6NUR] proteins with binding energies -7.7 kcal/mol, -8.5 kcal/mol, -7.9 kcal/mol and -8.3 kcal/mol respectively. The docking results were compared with human trial drugs such as hydroxychloroquine (HQC), favipiravir and lopinavir. The outcome gives information to show an excellent result on COVID-19 proteins. The docking results were illustrated in Table 5.

3.4. CONCLUSION

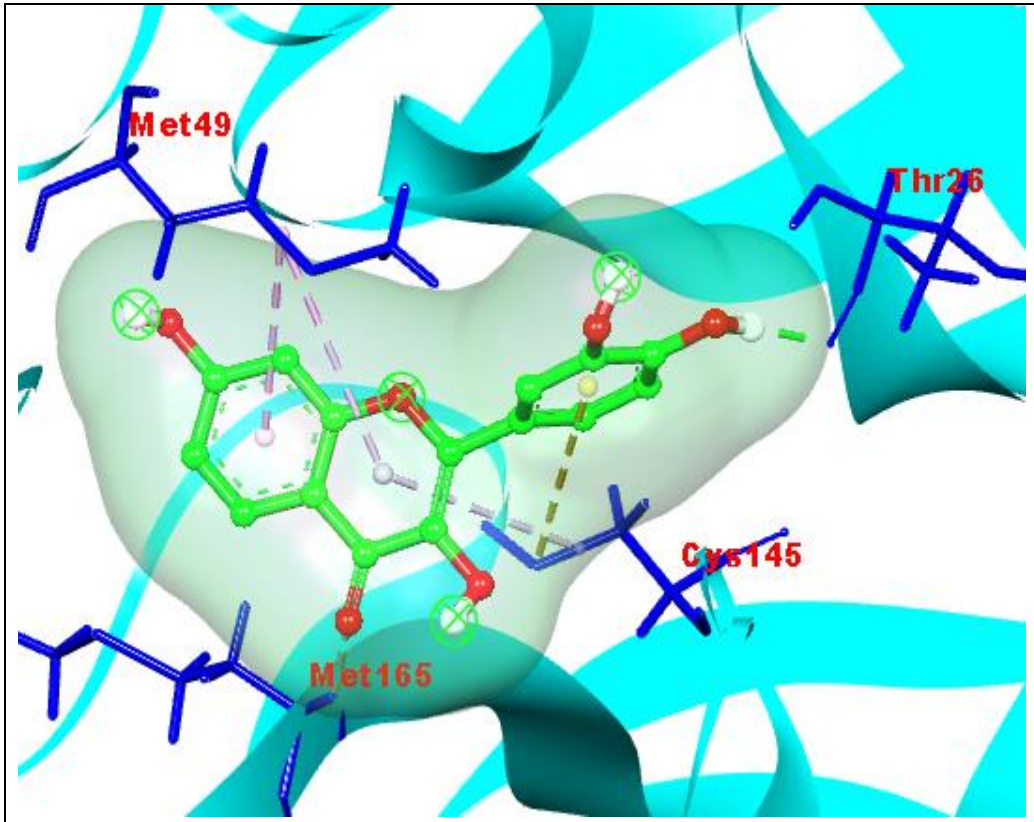
In the current work, three naturally occurring flavonoid compounds were evaluated for their *in vitro Covid-19* activities. Results of *Covid-19* study indicated that all the selected compounds having significant anti-viral activity against selected covid-19 receptor. Since the selectivity of the compounds is a very important parameter to become a good drug candidate, ADME prediction and docking studies also enhanced the biological importance of such compounds. As a result, it can be revealed that selected flavonoids derivatives are worthwhile to assess in further studies to develop new antiviral agents with higher potency and improved safety profile. The molecular docking study results reviewed that all selected flavonoids compounds showing excellent binding energy compared with FDA approved human trial drugs such as hydroxychloroquine, favipiravir

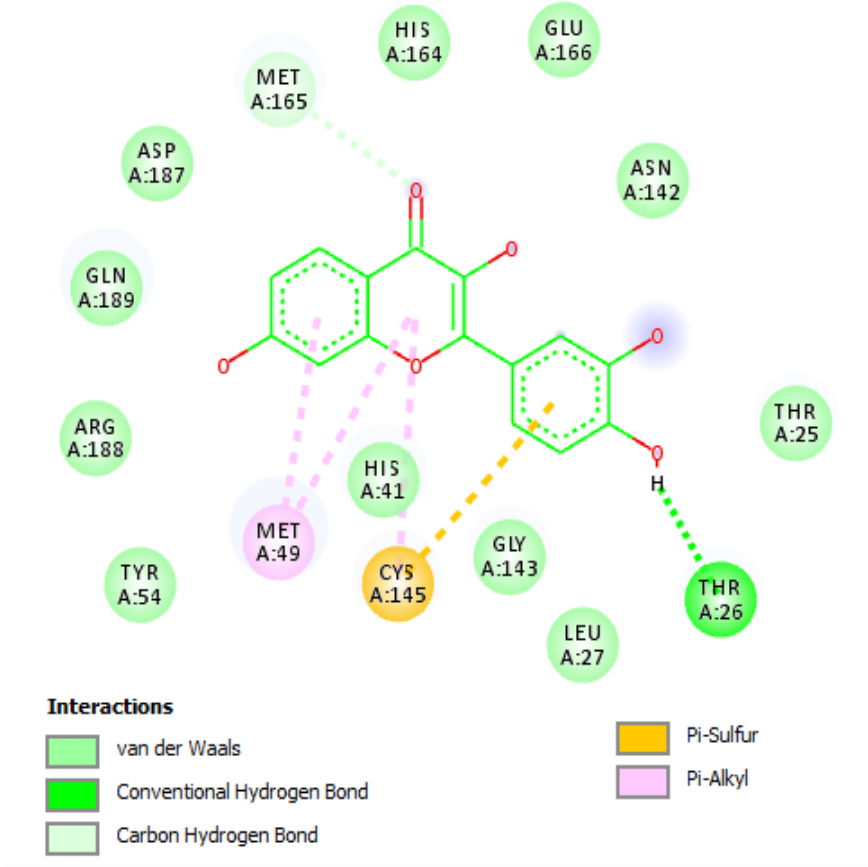
and lopinavir. In total the selected flavonoids ligands found to be with best results when compared to the standard drug used for against covid-19 viral activity.



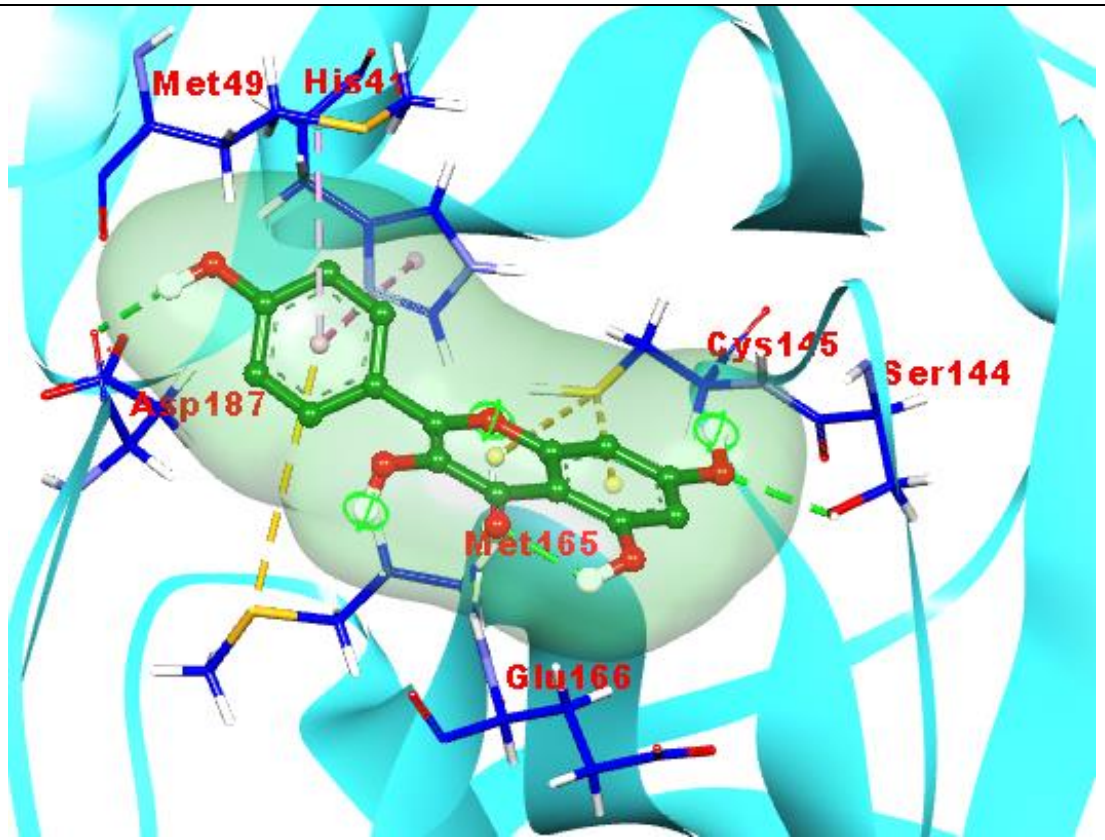


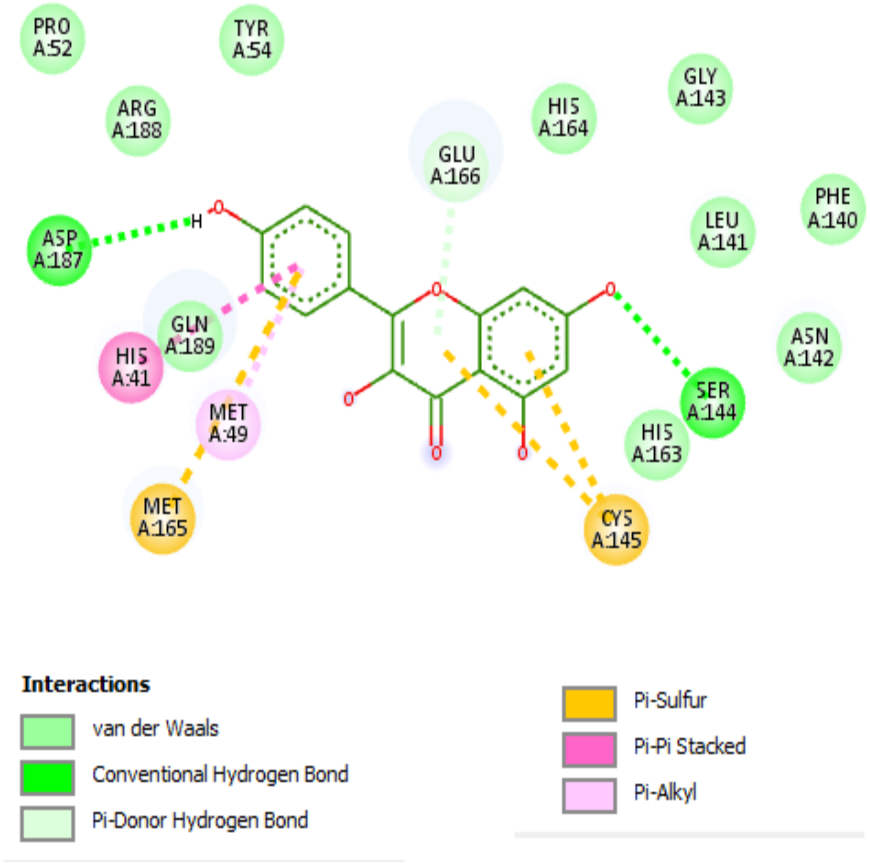
The 2D figures of the interactions of ligand 7A with the amino acids present in the protein 6LU7



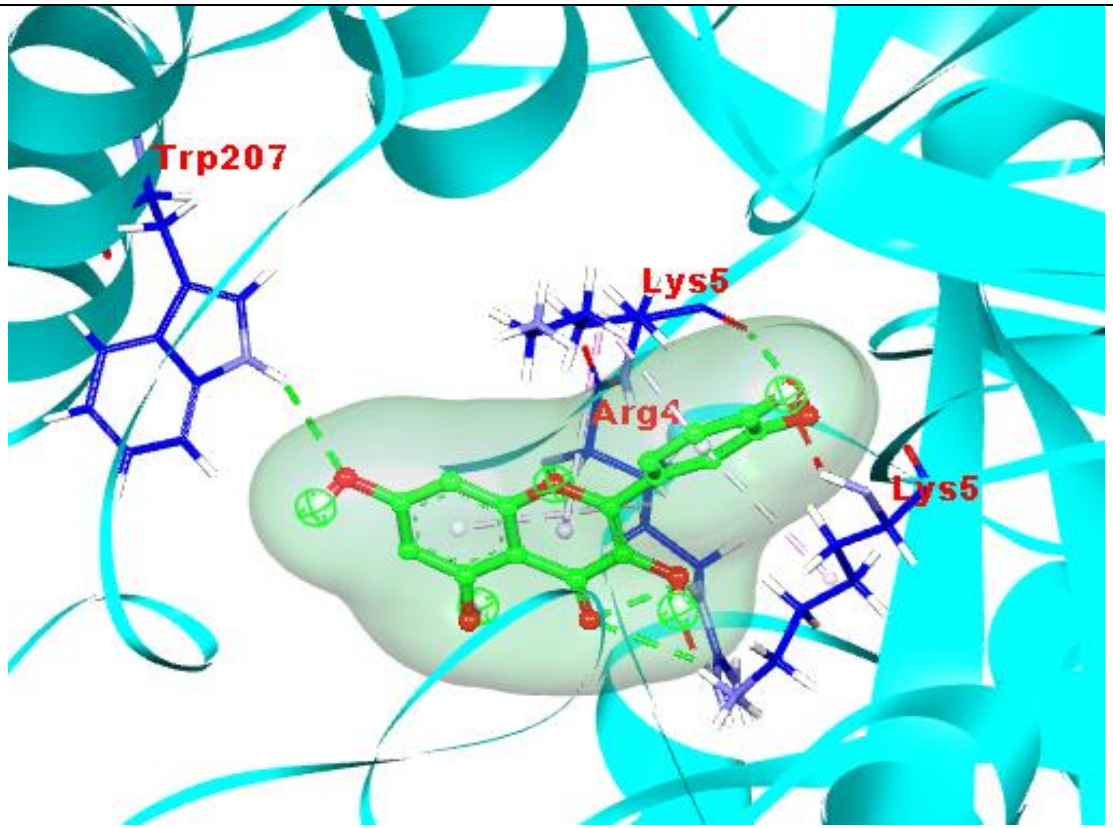


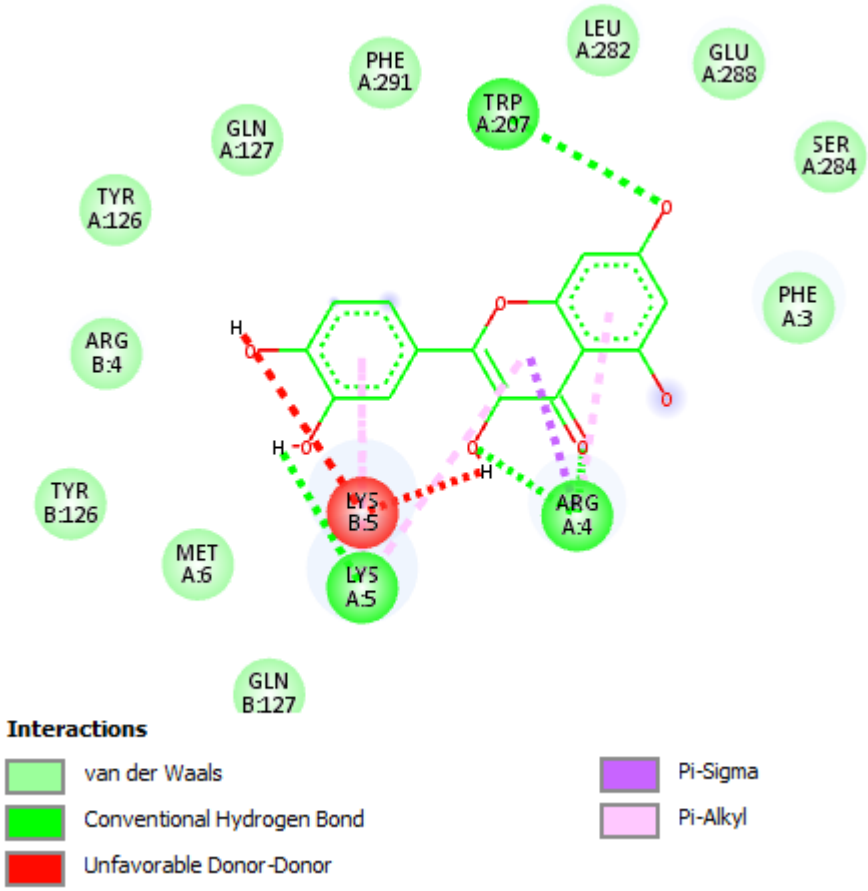
The 2D figures of the interactions of ligand 7B with the amino acids present in the protein 6LU7



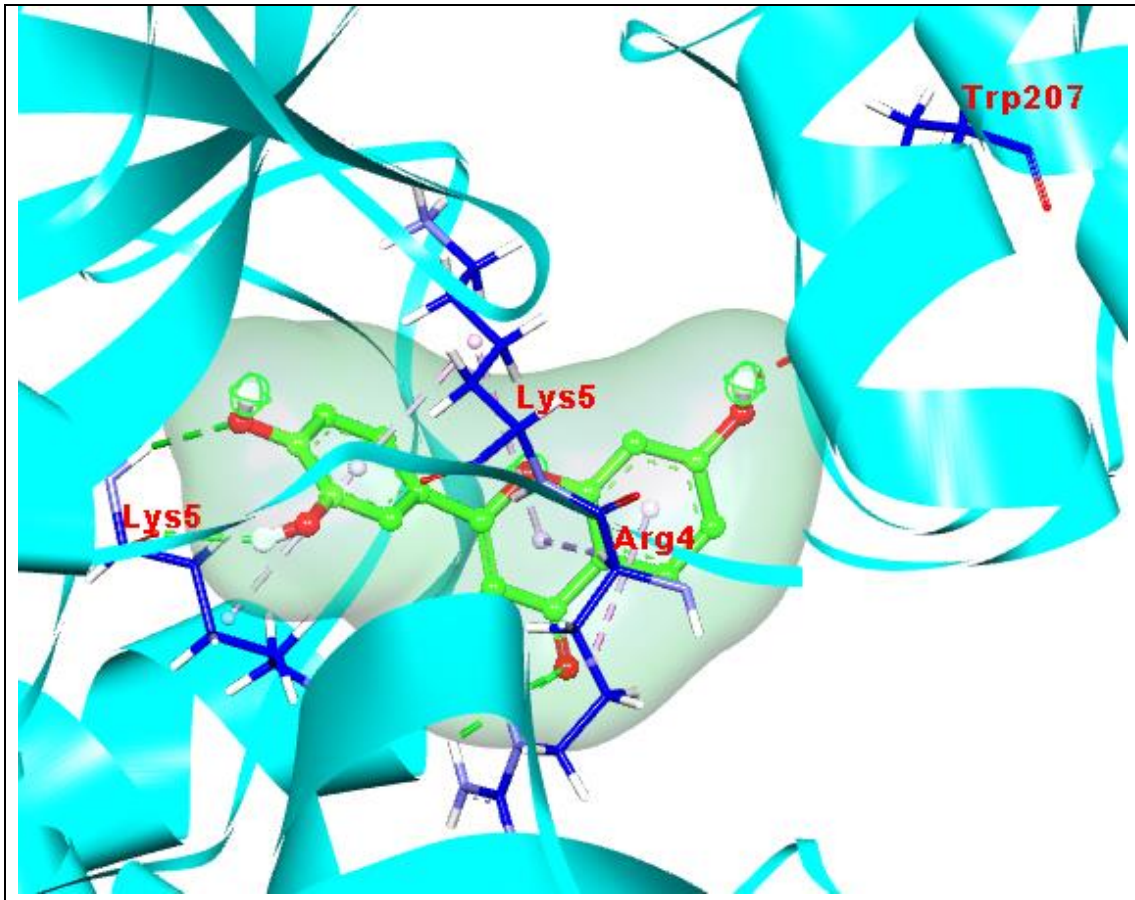


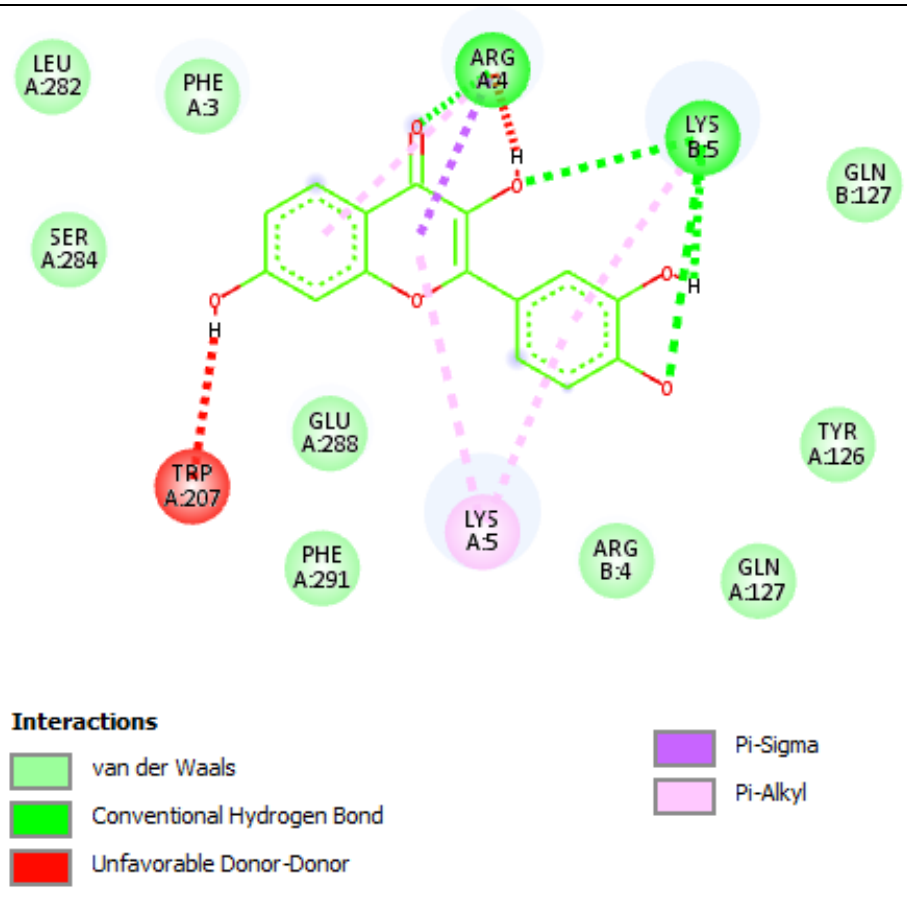
The 2D figures of the interactions of ligand 7C with the amino acids present in the protein 6LU7



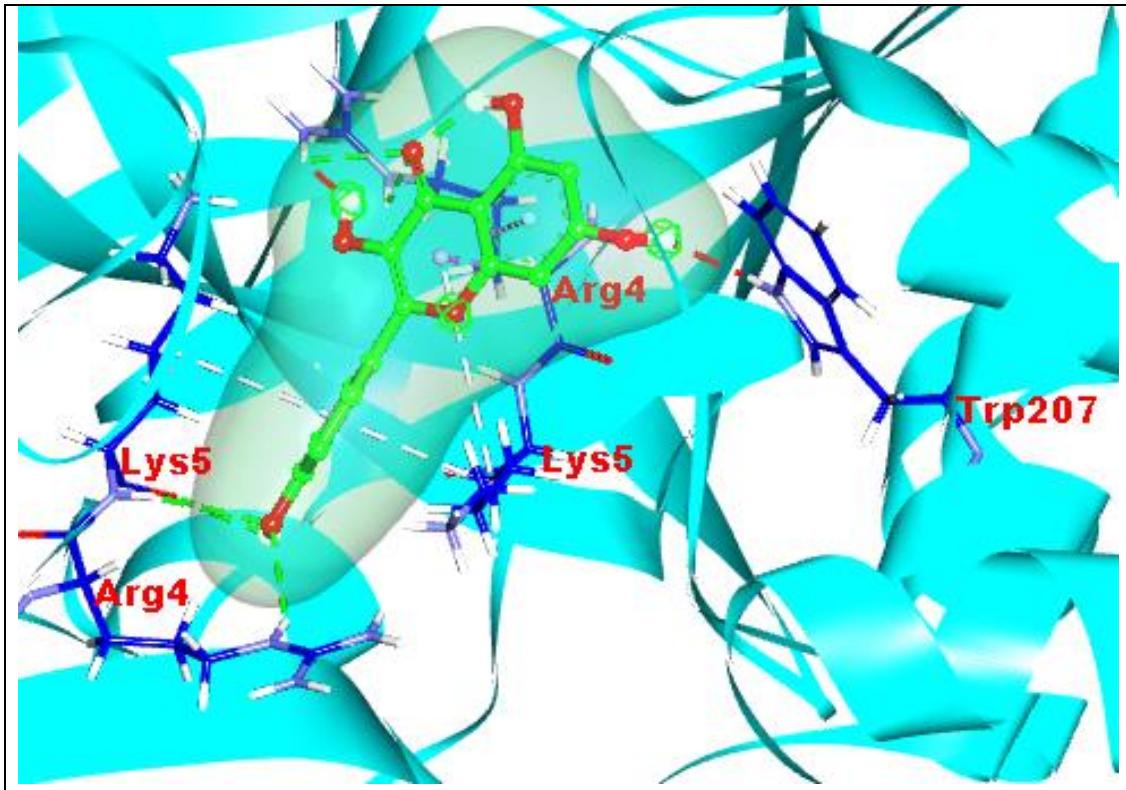


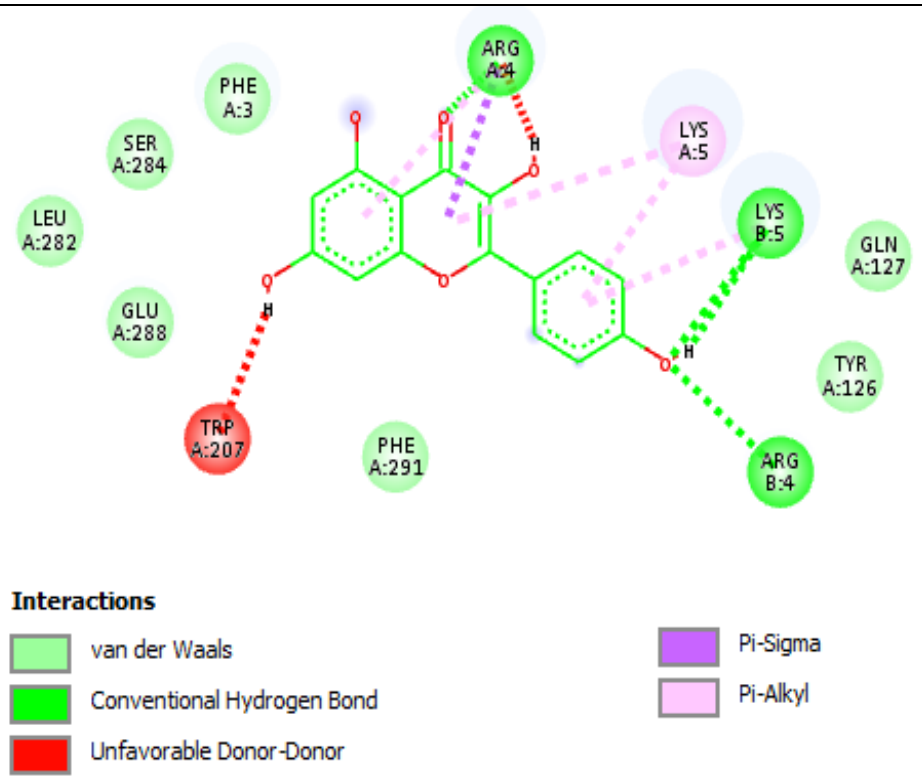
The 2D figures of the interactions of ligand 7A with the amino acids present in the protein 1UK4





The 2D figures of the interactions of ligand 7B with the amino acids present in the protein 1UK4





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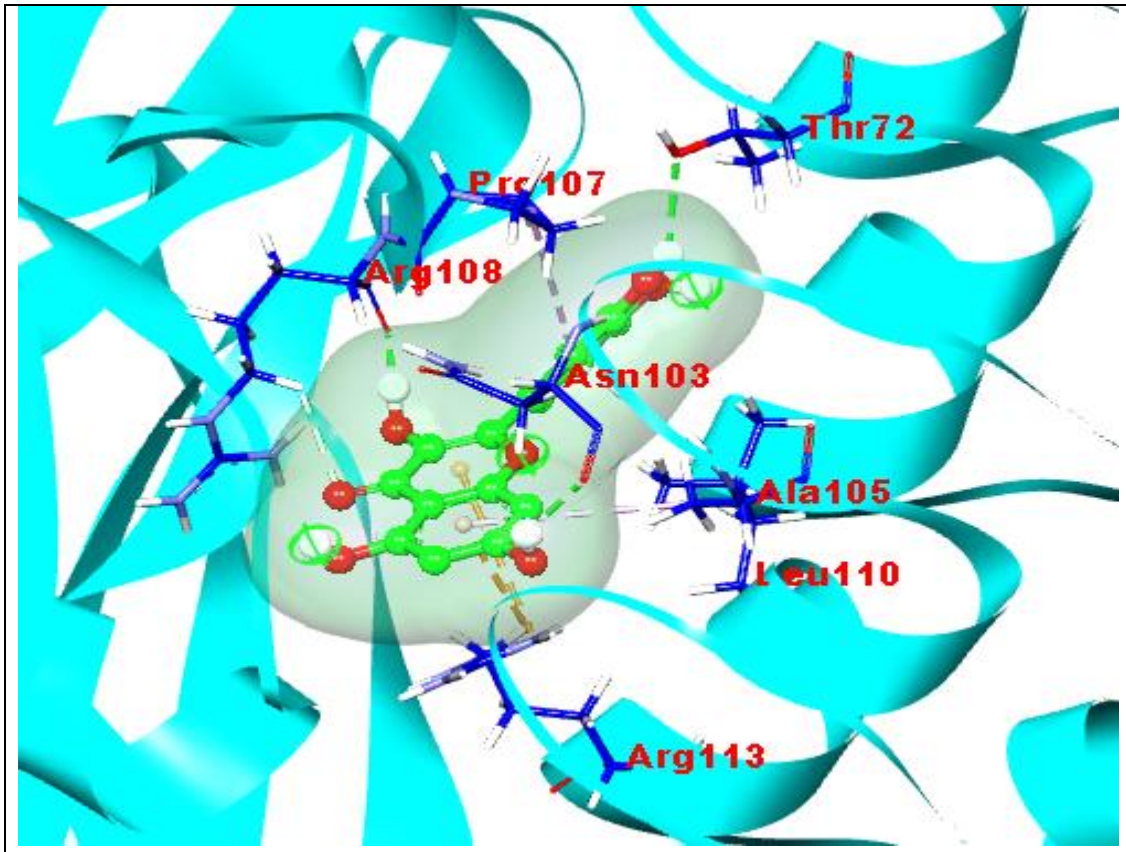

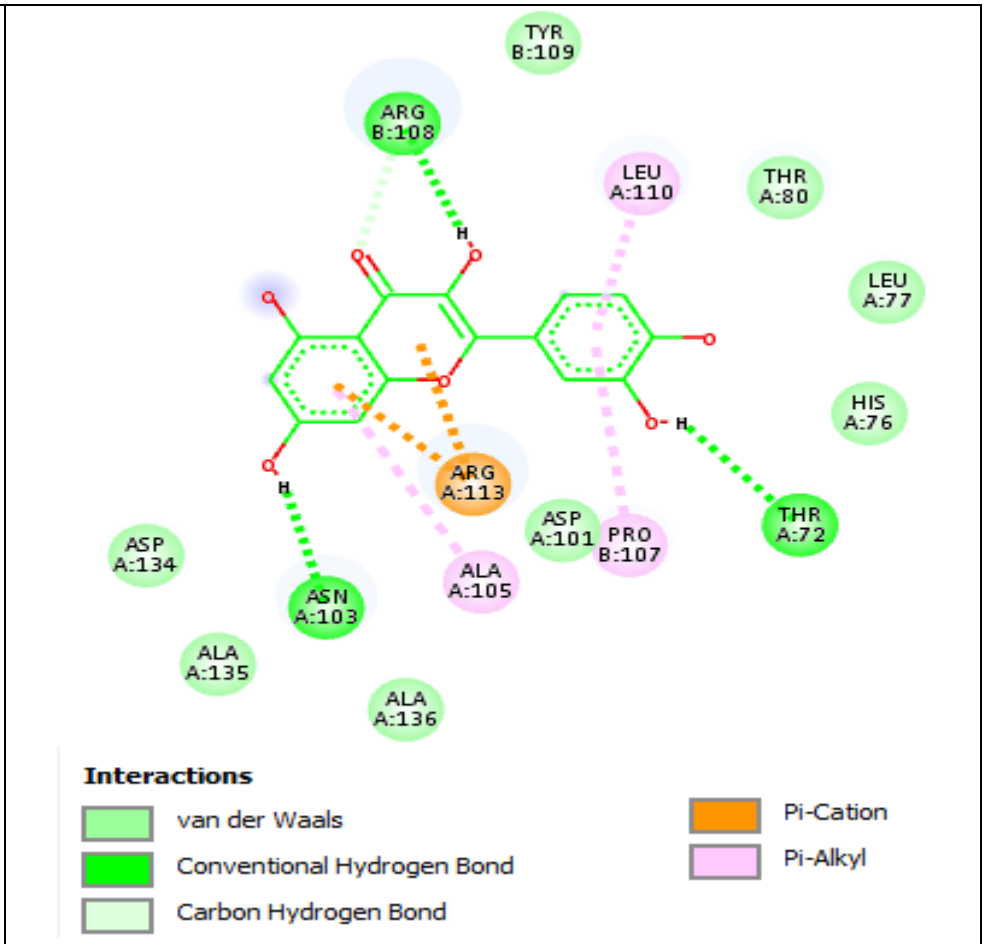

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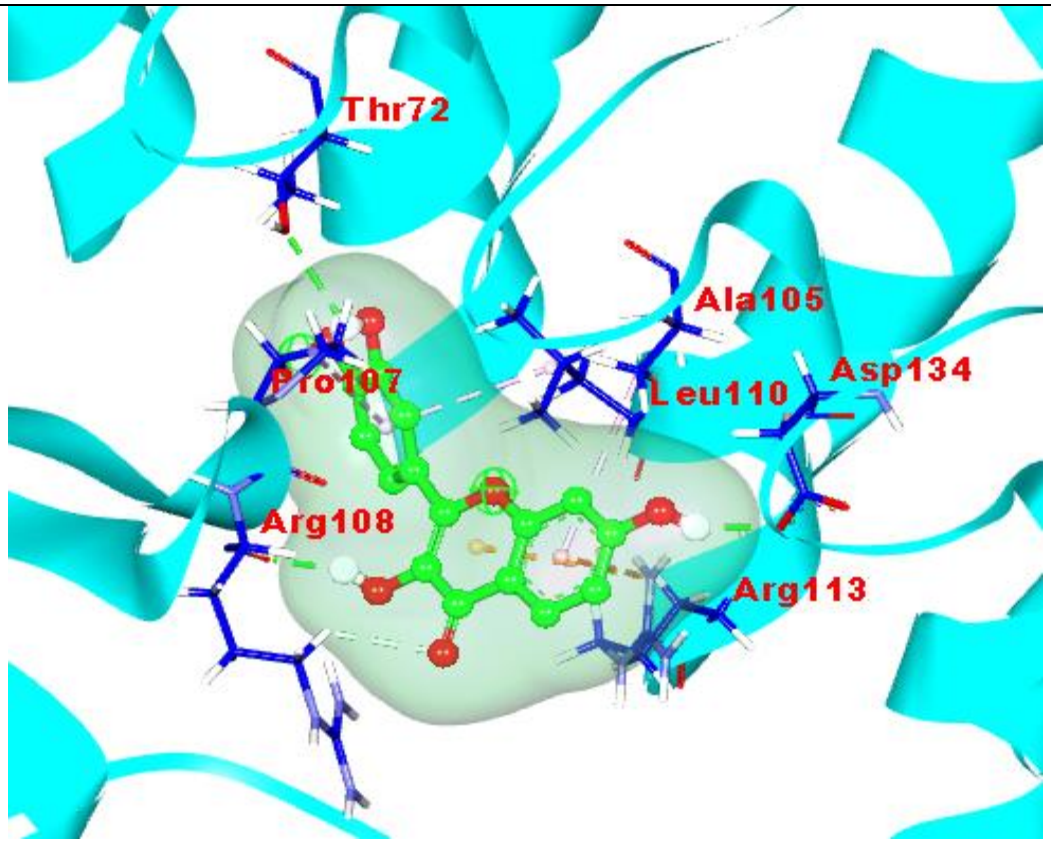

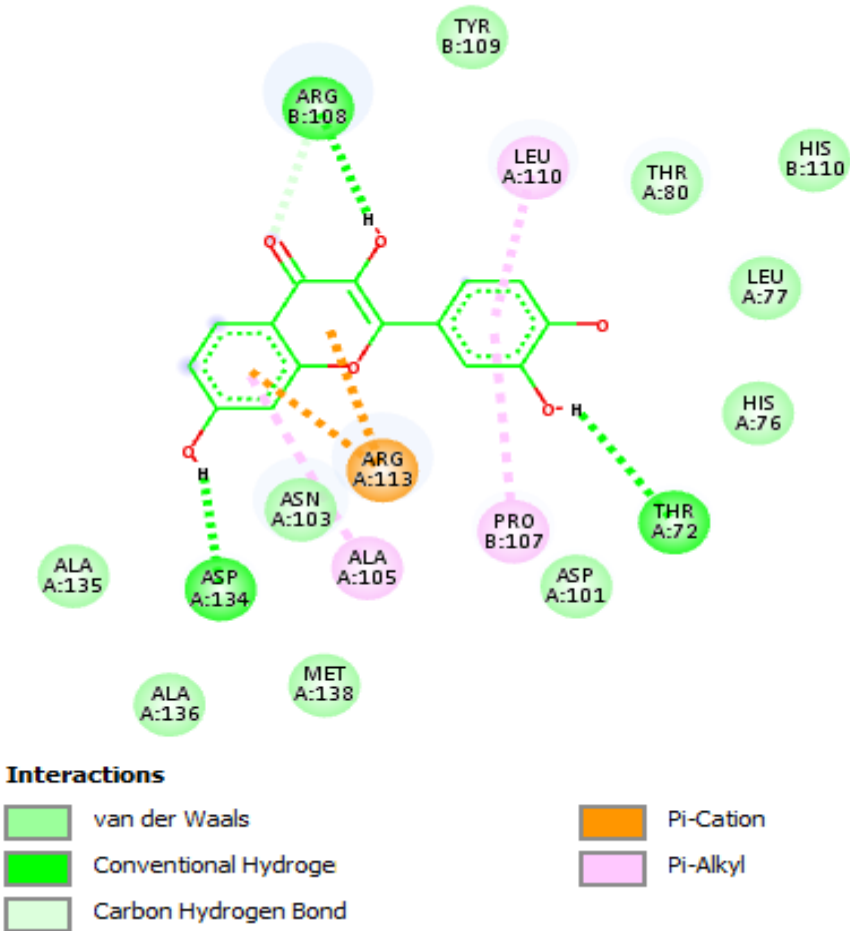

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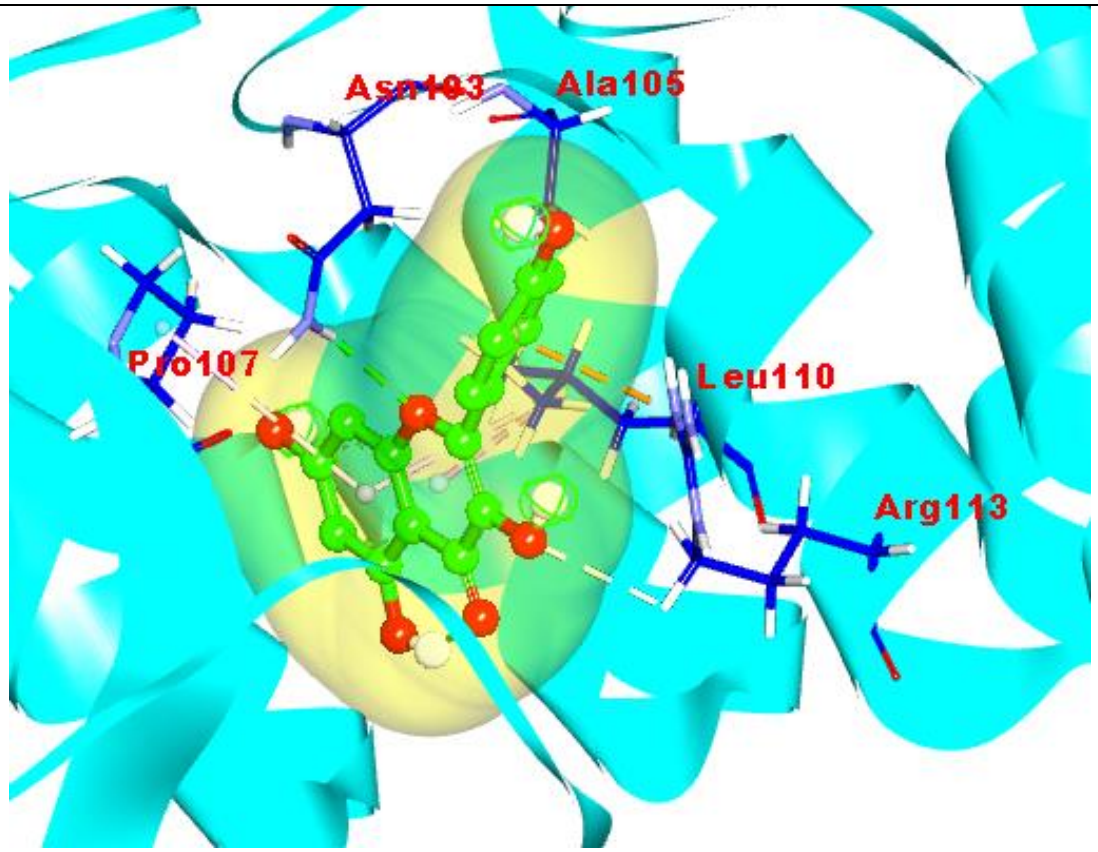

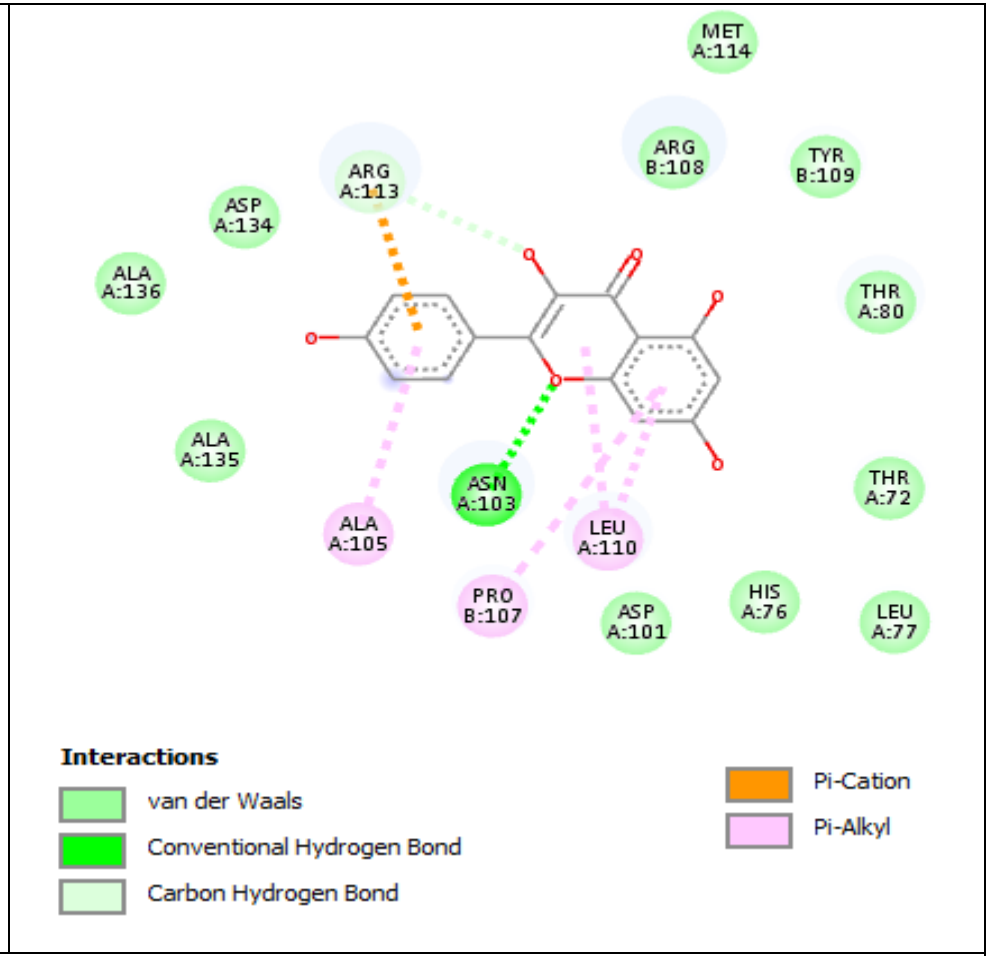

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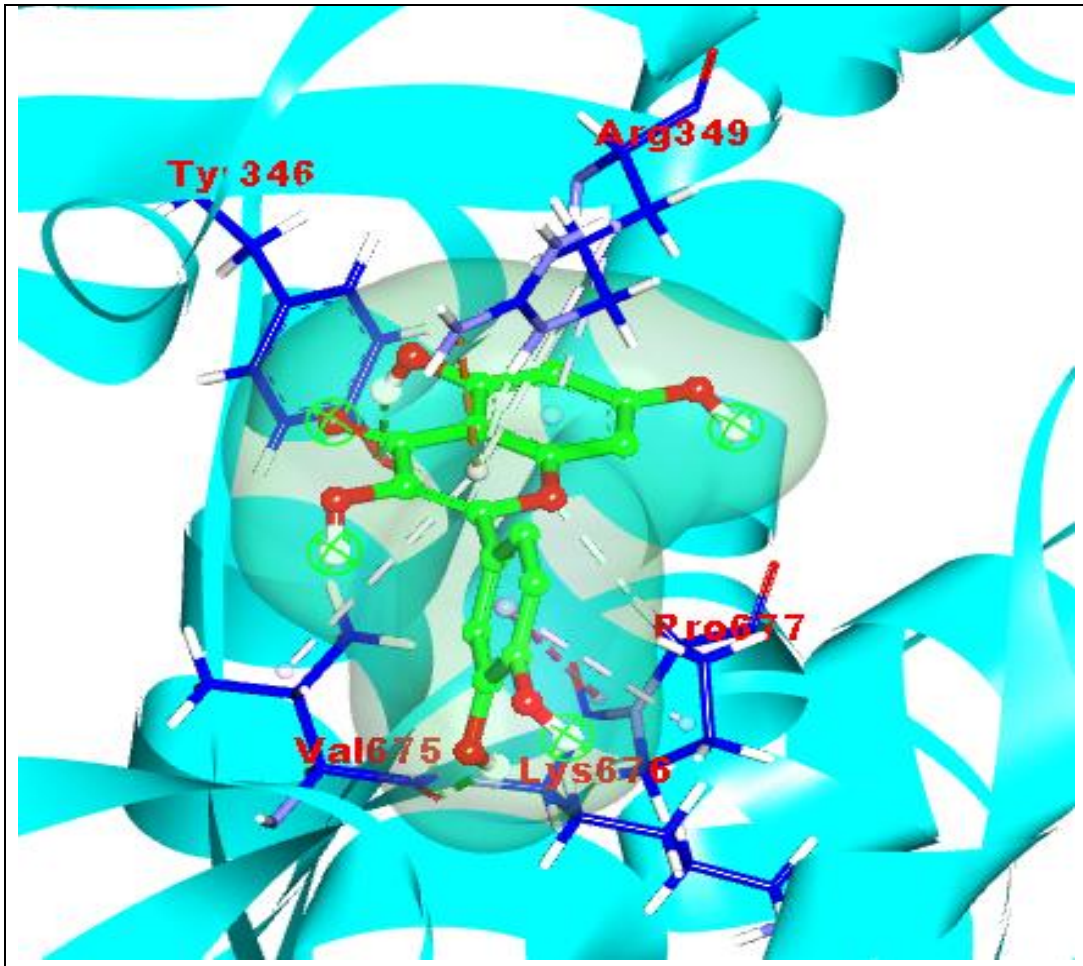

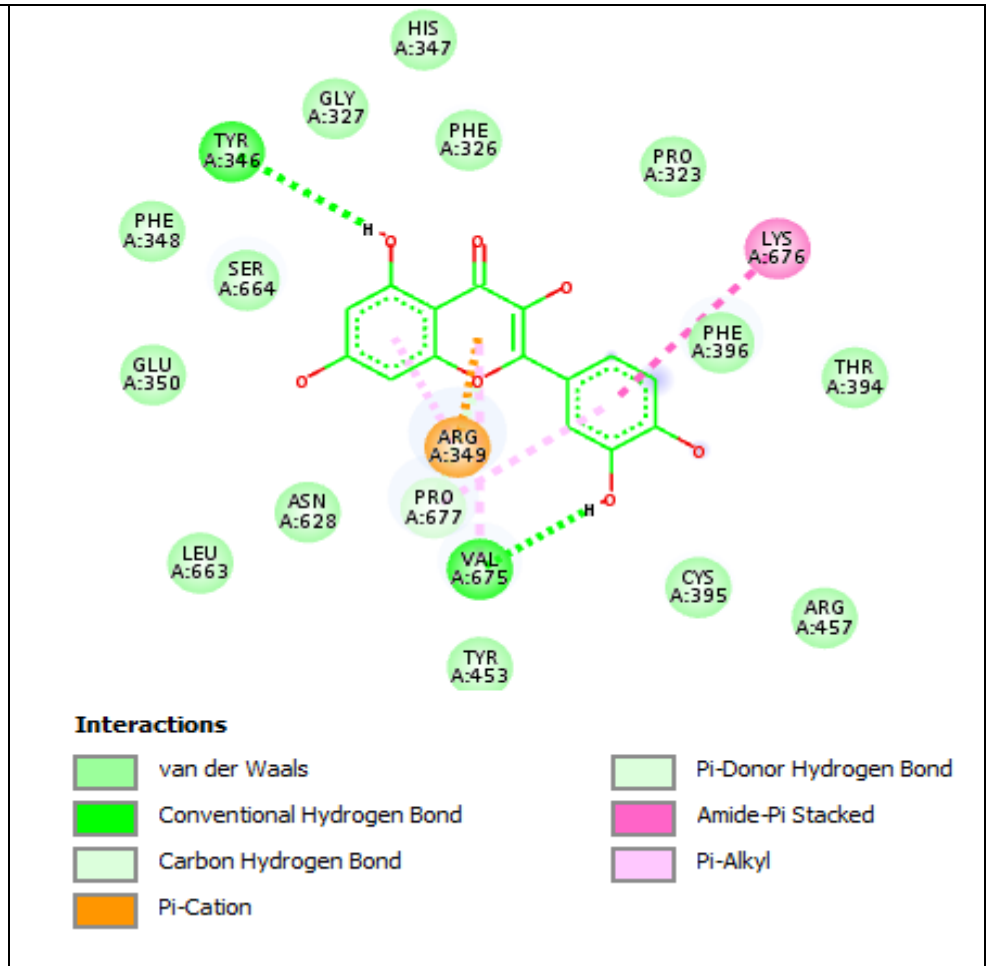

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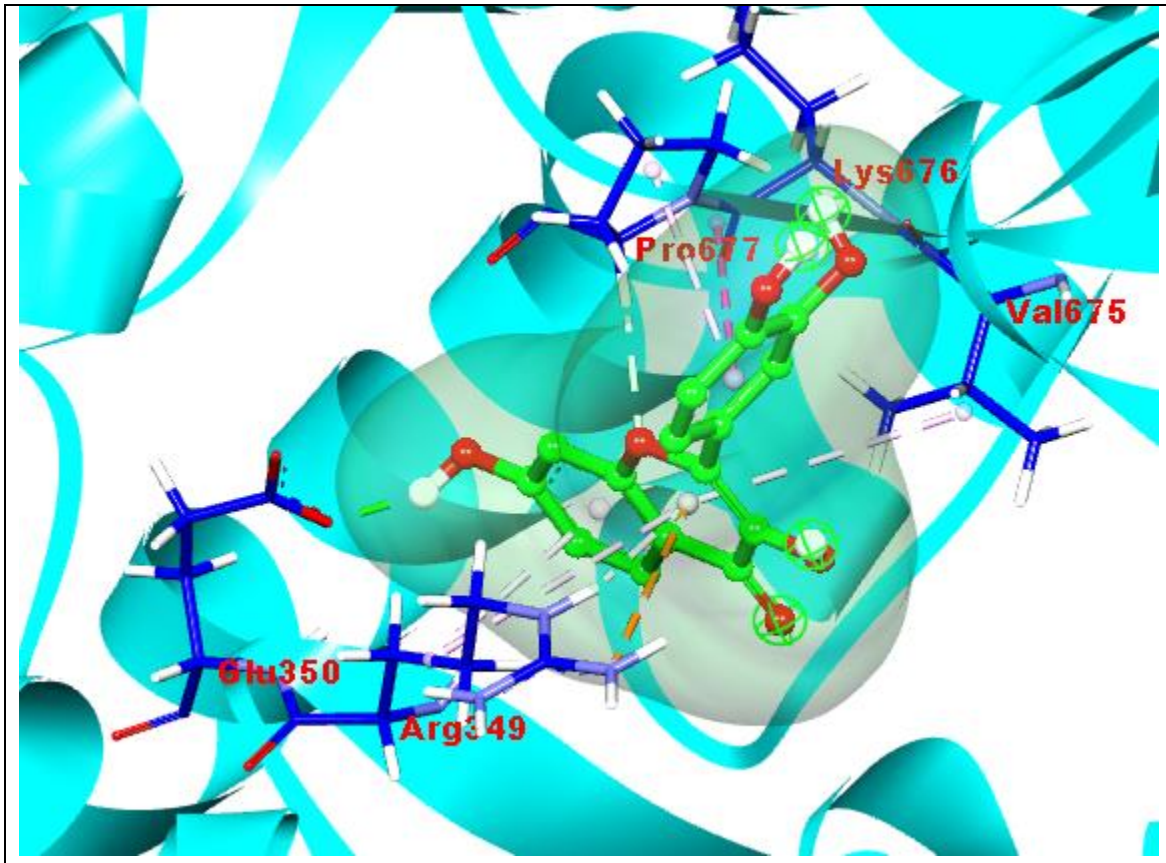

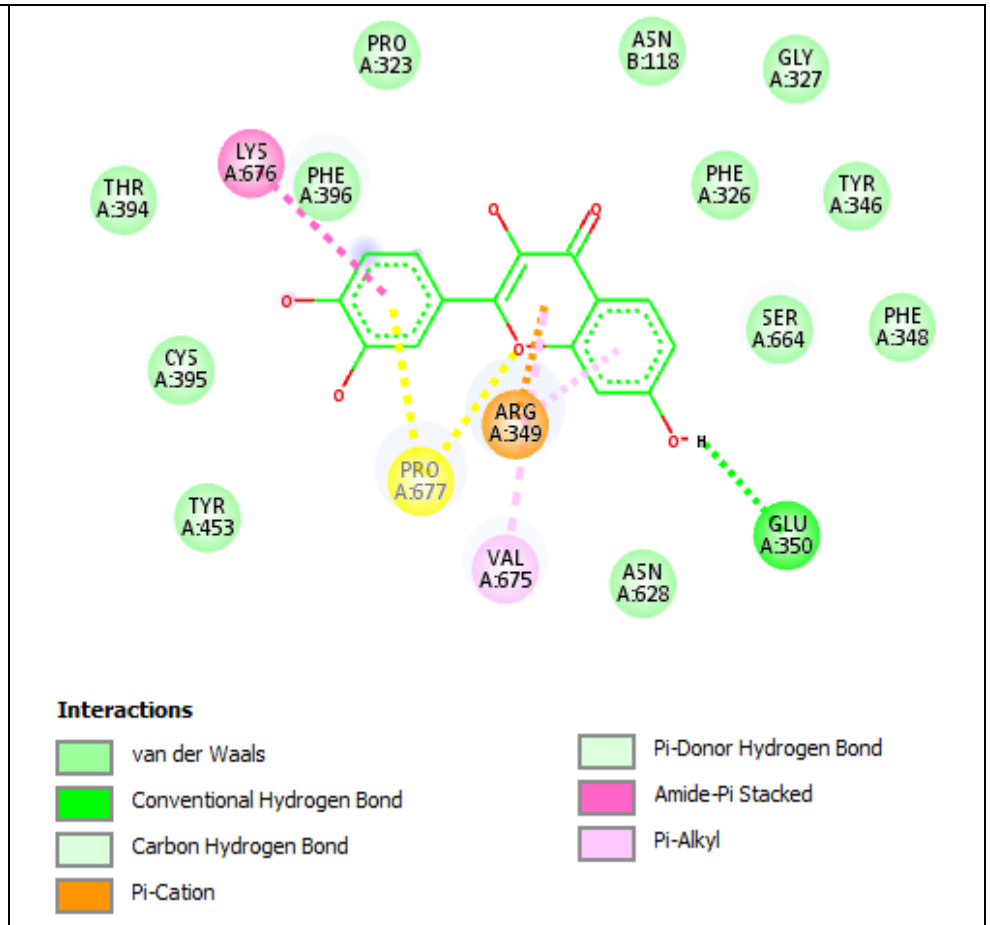

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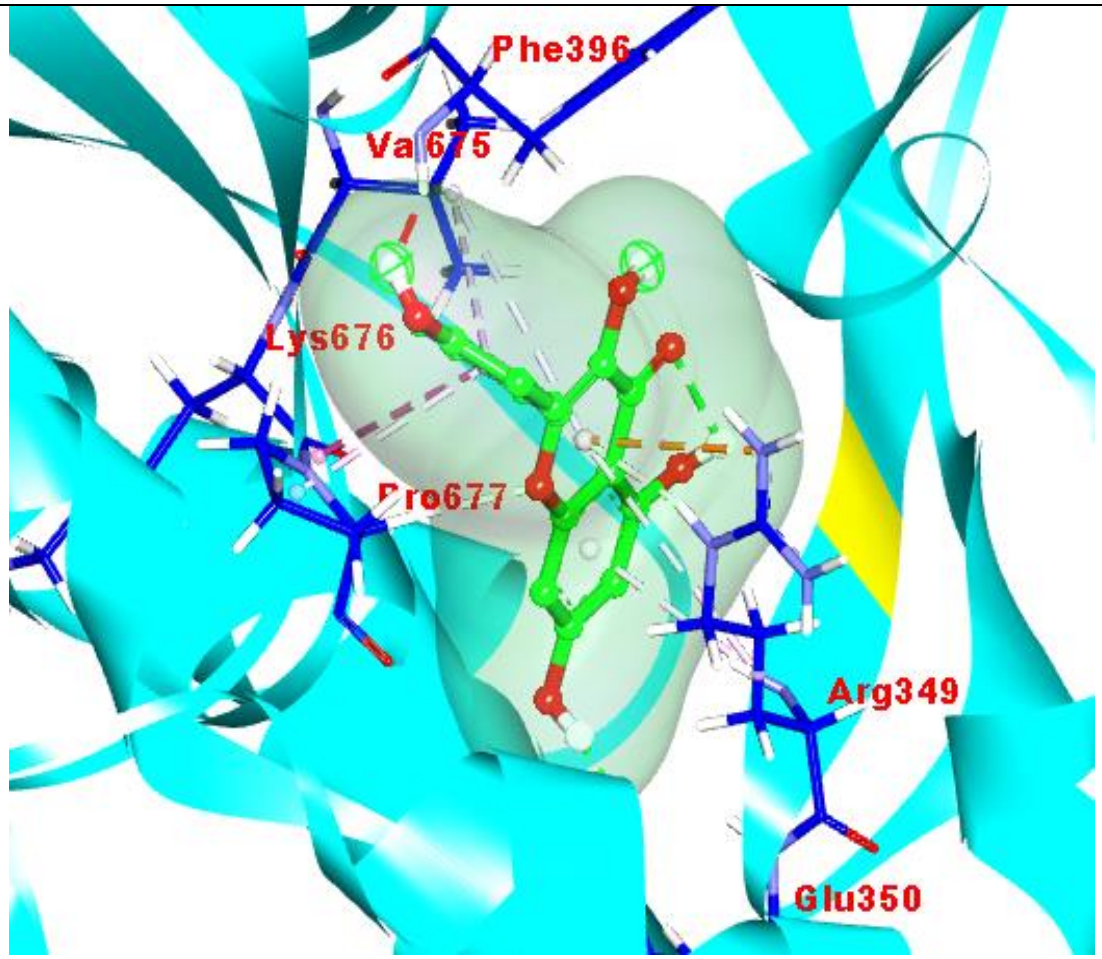

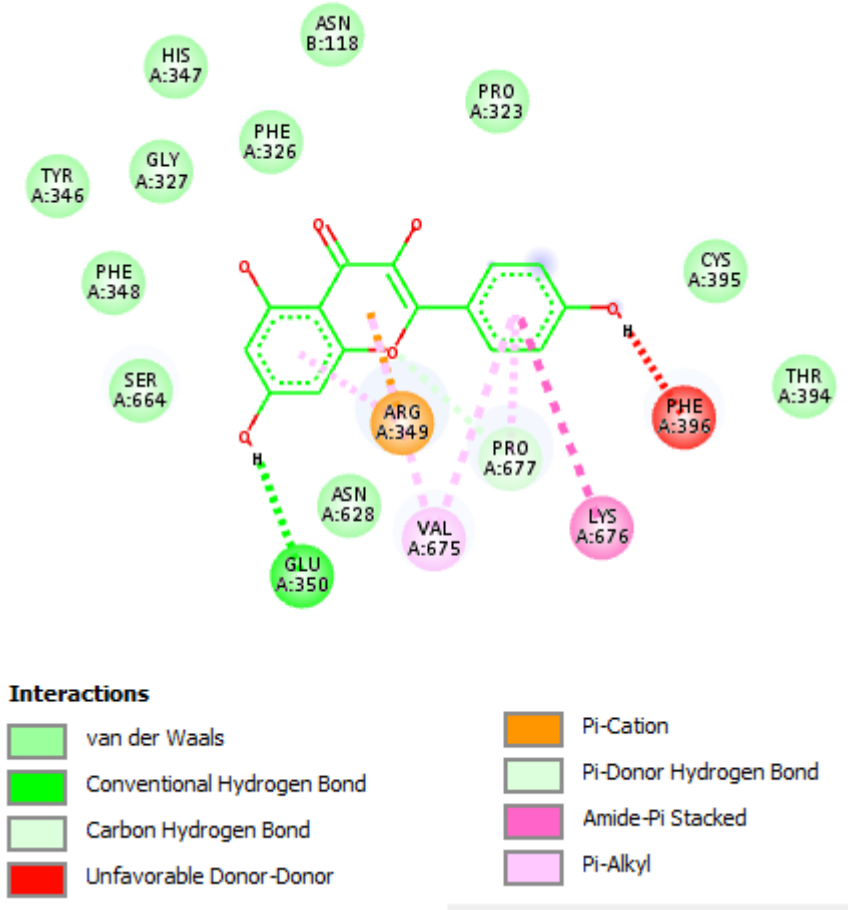

The 2D figures of the interactions of ligand 7C with the amino acids present in the protein 6NUR

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IN SILICO STUDIES ON INHIBITION EFFICENCY OF SOME NATURALLY OCCURRING FLAVONOIDS AGAINST SARS COV-2 RECEPTORS

Dissertation submitted to the Christ College (Autonomous) in partial fulfilment of the requirement for the Degree of

BACHELOR OF SCIENCE

IN

CHEMISTRY

Submitted by

SREERAG SHANIL

Reg. No: CCAUSCH034

2020-2023

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DECLARATION

I, SREERAG SHANIL (Reg.No.CCAUSCH034) do hereby declare that, this dissertation work entitled "**IN SILICO STUDIES ON INHIBITION EFFICENCY OF SOME NATURALLY OCCURRING FLAVONOIDS AGAINST SARS COV-2 RECEPTORS" s**ubmitted to the University of Calicut in Partial Fulfilment of the requirement for the award of degree of Bachelor of Science was carried under the guidance of Dr.Tom Cherian, Assistant professor, Department of Chemistry, Christ College, Irinjalakuda and it is a record of original project work carried out by me and it has not previously formed the basis for the award of, any degree, Diploma fellowship or other similar title of recognition by any other university or institutions.

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CERTIFICATE

This is to certify that SREERAG SHANIL (Reg.No.CCAUSCH034) has carried out a project work entitled **"IN SILICO STUDIES ON INHIBITION EFFICENCY OF SOME NATURALLY OCCURRING FLAVONOIDS AGAINST SARS COV-2 RECEPTORS"** is an authentic record of the research project carried out by my supervision and guidance in the P.G & Research Department of Chemistry, Christ College, Irinjalakuda. It is further certified that this project report has not previously formed the basis for the award of any Degree, Diploma, Fellowship or other similar title of recognition by any other university or Institutions.

Dr. Tom Cherian

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SREERAG SHANIL

CONTENTS

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I, SUSMERA P S (Reg.No.CCAUSCH035) do hereby declare that, this dissertation work entitled "**IN SILICO STUDIES ON INHIBITION EFFICENCY OF SOME NATURALLY OCCURRING FLAVONOIDS AGAINST SARS COV-2 RECEPTORS" s**ubmitted to the University of Calicut in Partial Fulfilment of the requirement for the award of degree of Bachelor of Science was carried under the guidance of Dr.Tom Cherian, Assistant professor, Department of Chemistry, Christ College, Irinjalakuda and it is a record of original project work carried out by me and it has not previously formed the basis for the award of, any degree, Diploma fellowship or other similar title of recognition by any other university or institutions.

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Asst. Professor in Chemistry

CERTIFICATE

This is to certify that SUSMERA P S (Reg.No.CCAUSCH035) has carried out a project work entitled **"IN SILICO STUDIES ON INHIBITION EFFICENCY OF SOME NATURALLY OCCURRING FLAVONOIDS AGAINST SARS COV-2 RECEPTORS"** is an authentic record of the research project carried out by my supervision and guidance in the P.G & Research Department of Chemistry, Christ College, Irinjalakuda. It is further certified that this project report has not previously formed the basis for the award of any Degree, Diploma, Fellowship or other similar title of recognition by any other university or Institutions.

Dr. Tom Cherian

ACKNOWLEDGEMENT

I extend my sincere and heartfelt gratitude to my project guide Dr. Tom Cherian, Department of chemistry, Christ College, Irinjalakuda for his valuable and inspiring guidance, critical assessment and constant encouragement at all stages of this project. I am greatly indebted to him for the completion of this work in the specified period.

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Above all I humbly thank God Almighty, whose sustaining grace has been sufficient for me to complete this endeavour.

SUSMERA P S

CONTENTS

IN SILICO STUDIES ON INHIBITION EFFICENCY OF SOME NATURALLY OCCURRING FLAVONOIDS AGAINST SARS COV-2 RECEPTORS

Dissertation submitted to the Christ College (Autonomous) in partial fulfilment of the requirement for the Degree of

BACHELOR OF SCIENCE

IN

CHEMISTRY

Submitted by

SUSMITHA K

Reg. No: CCAUSCH036

2020-2023

P.G AND RESEARCH DEPARTMENT OF CHEMISTRY

CHRIST COLLEGE, IRINJALAKUDA

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I, SUSMITHA K (Reg.No.CCAUSCH036) do hereby declare that, this dissertation work entitled "**IN SILICO STUDIES ON INHIBITION EFFICENCY OF SOME NATURALLY OCCURRING FLAVONOIDS AGAINST SARS COV-2 RECEPTORS" s**ubmitted to the University of Calicut in Partial Fulfilment of the requirement for the award of degree of Bachelor of Science was carried under the guidance of Dr.Tom Cherian, Assistant professor, Department of Chemistry, Christ College, Irinjalakuda and it is a record of original project work carried out by me and it has not previously formed the basis for the award of, any degree, Diploma fellowship or other similar title of recognition by any other university or institutions.

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ACKNOWLEDGEMENT

I would like to begin by expressing gratitude to God Almighty for all his blessings.

With great pleasure, I express my sincere gratitude to Dr. Jibin A.K, Assistant Professor, Department of Chemistry, Christ College (Autonomous), Irinjalakuda, for his dynamic effort in guiding and instructing me for the completion of this work successfully.

I acknowledge my humble thanks to teachers and non-teaching staffs for their valuable suggestions and help.

Last but not the least, I express thanks to my family, classmates, and friends for being with me, especially when I need them.

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ABSTRACT

Bilimbi, being a fruit containing high oxalic acid content in it, is taken for investigation. This work focuses on two age groups of bilimbi, ripened and half ripened is observed to have significant difference in its oxalic acid content**.**

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ABSTRACT

Bilimbi, being a fruit containing high oxalic acid content in it, is taken for investigation. This work focuses on two age groups of bilimbi, ripened and half ripened is observed to have significant difference in its oxalic acid content**.**

CONTENTS

INTRODUCTION

Averrhoa bilimbi, commonly known as bilimbi, belongs to the family of the Oxalidaceae. It is widely cultivated in the tropics and its origins are not yet clear. Nevertheless, Correa (1926) reported that it is native of India. In our region we call it as “irumbanpulli”. Bilimbi is a small tree up to 15 meters high. Fruits are fairly cylindrical with five broad rounded longitudinal lobes, and produced in clusters. During maturity stage occurs the maximum increase in fruits weight and dimensions, and their external green colour changes into light yellow.

Mineral constituents of half ripen Averrhoa bilimbi fruits, Nitrogen, nitrate, phosphorous, potassium, calcium, magnesium, sulphur and sodium were found to be major minerals while zinc, ferrous, copper, manganese, molybdenum and boron were minor elements. Phosphorus content of the fruit is maximum while nitrate content is lowest in case of major elements, while ferrous is maximum i.e. 33.12 ± 1.34 and molybdenum is lowest (0.04 ± 0.005) in minor elements.

The oxalic acid levels in bilimbi ranged between 8.57 and 10.32 mg/g. These high levels of oxalic acid is found in bilimbi. Oxalic acid has been identified as the main acid in carambola and in bilimbi. Other foods also have high levels of oxalic acid, such as spinach (8.22 mg/g), cocoa powder (4.5 mg/g) and tealeaves (3.8-14.5 mg/g).

Ripe bilimbi fruits have higher vitamin C content than half-ripe ones. This pattern has also been observed on guava and camu-camu. In other fruits, like acerola, the opposite happens: thehighest levels of vitamin C are found in half-green and green fruits. The levels of vitamin C inripe and half-ripe bilimbi fruits varied from 20.82 to 60.95 mg/100g. The vitamin C levels in ripe and half-ripe bilimbi harvested in the same season were statistically different. Ripe fruits harvested during dry season had the highest vitamin C level. This result may have been influenced by climatic factors. As expected, during the dry season, an increase of photosynthetic activity (induced by rising solar radiation and reduced average seasonal rainfall)produces higher levels of vitamin C, since this vitamin is synthesised from hexose sugar precursors. In spite of the low levels of vitamin C in bilimbi, the ripe fruit has significant amount of this vitamin. Therefore, the medicinal use of this fruit against scurvy, which was recommended by Correa and Wong & Wong, can be justified.

Based on results it may be concluded that maturity stage influenced on physicochemical characteristics of bilimbi fruit and ripe bilimbi harvest during dry season showed the lowest levels of oxalic acid and the highest levels of SST and vitamin C.

Therefore, it is recommended that this fruit should be consumed when it is completely ripe. Averrhoa bilimbi fruit is a good source of minerals such as potassium, calcium, phosphorous and iron. They are low in calorie, sodium and lipids which qualifies it as an excellent source of natural antioxidants and minerals. Physical properties and dimensions of mature Averrhoa bilimbi fruits are ideal as green vegetable for human consumption. Overall composition of mineral elements suggests Averrhoa bilimbi fruit is good source of minerals and a potential fruit to be popularised for diet.

Averrhoa bilimbi (Oxalidaceae) is widely distributed and cultivated throughout tropical countries for its fruits. Parts such as leaves bark and fruits are widely used in medicine as a folk remedy for many symptoms. This study provides morphological and biochemical characteristics of half-ripen bilimbi fruits. During present study physical and chemical properties of Bilimbi fruits were studied at half-ripen stage for potential benefits based on its mineral content.

Phosphorus content of the fruits was higher at half-ripen stage i.e. 39 ± 1.7%, while in case of minor elements, Molybdenum is present in least amount i.e. 0.04 ± 0.05 ppm. This Chemical study reveals that the fruit is good source of minerals such as Potassium, Phosphorus, Nitrogen, Calcium, Magnesium and Iron suggesting its use as a potential fruit.

PROPERTIES

Ripe bilimbi fruits have thin skin, yellowish-green colour, soft texture and a peculiar smell, which resembles the one of carambola, a fruit of the same botanical family. Half-ripe fruits have firm texture and imperceptible smell. Bilimbi is a small tree up to 15 meters high. Fruits are fairly cylindrical with five broad rounded longitudinal lobes, and produced in clusters.

Table 1: Physical features of mature fruits of *Averrhoa bilimbi* L.

Sr. No.	Parameters studied	Analysis
01	Length of fruit (cm)	6.1 ± 0.38
02	Diameter of fruit (cm)	2.1 ± 0.16
03	Length/diameter ratio	2.8 ± 0.32
04	Number of ridges	5.0 ± 0.0
05	Length of ridges (cm)	5.7 ± 0.32
05	Width of ridges (cm)	0.4 ± 0.05
06	Weight of fruit (g)	18.6 ± 2.17
07	Moisture Content of fruit (%)	96.9 ± 0.06
08	Dry weight of fruit (g)	0.55 ± 0.05
09	Number of seeds/ fruit	7.7 ± 2.45
10	Weight of seeds(g)	0.16 ± 0.08

(n=10; mean ± SD)

USES

Bilimbi fruits are very sour, and used in the production of vinegar, wine, pickles and in the preparation of Indian dishes. The mature fruits can be eaten in natura or processed into jams and jellies. Medicinal uses are attributed to bilimbi, which include mixtures against cough, mumps, rheumatism, pimples and scurvy.

The fruit juice has high levels of oxalic acid, and therefore may be used to remove iron-rust stains from clothes and to impart shine to brassware.

LITERATURE REVIEW

Oxalic acid has been identified as the main acid in carambola and in bilimbi. The oxalic acid levels in Bilimbi ranged between 8.57 and 10.32 mg/g. These are the high levels of oxalic acid found in bilimbi. Other foods that has high levels of oxalic acid are spinach (8.22 mg/g), cocoa powder (4.5 mg/g) and tea leaves (3.8-14.5 mg/g).

Chemical characteristics in ripe and half-ripe bilimbi fruits harvested on dry and rainy seasons.

	Dry Season*		Rainy Season**	
	ripe fruits	half-ripe fruits	ripe fruits	half-ripe fruits
Oxalic acid (g/100g)	8.57 d	9.33 bd	9.82 bc	10.32 ab
Vitamin C (mg/100g)	60.95 a	32.23 cd	36.68 bc	20.82 de
TSS (° Brix)	5.06 a	4.34 bc	4.64 ab	3.94 cd

METHODS FOR THE DETERMINATION OF OXALIC ACID CONTENT IN BILIMBI

Many methods are used for the determination of oxalic acid content in bilimbi. And some of them are mentioned below.

METHOD 1:

15g of bilimbi is taken and crushed in to fine pulp. Then the pulp is transferred to a beaker and add 50 mL of dilute sulphuric acid to it and boil it for 2 minutes. Cool the contents and filter it in to a 100 mL measuring flask and make up to 100 mL. 20 ml of this solution is taken and transferred in to a conical flask. To it add 20 ml of dilute sulphuric acid and the mixture is heated to about 60 degrees Celsius. It is then titrated against 1/20 N KMnO4 solution from the burette. An appearance of permanent light pink colour indicates the end point.

METHOD 2:

2 gram of the sample is taken in a 250 ml standard flask. It is then mixed with 10 ml of 6 N HCl and 190 ml water. It is then made up in to 250 ml and filtered. 50 ml of filtrate is taken in a conical flask and 10 ml of 6 N HCl is added in to it. It is then evaporated in a water bath to half of its volume. The solution is filtered and the precipitate is washed. The collected precipitate is then made up to 125 ml. To these 2 to 3 drops of methyl red indicator is added. Concentrated ammonia is added drop wise till the solution turns in to faint yellow colour. It is the heated at 90 degrees Celsius and cooled and filtered. It is then boiled and 10 ml of 5 % CaCl2 is added and stirred. Then leave the solution for overnight. It is then filtered and precipitate is washed in hot water. Dissolve this precipitate in 30 ml of water and concentrated sulphuric acid in the ratio 3:1. It is then heated at 70 degrees Celsius for 10 minutes and cooled. This solution is titrated against 1/20 N $KMnO_4$ to the end point which is indicated by the permanent colour change.

METHOD 3:

Acid – base titration method is used here. Bilimbi is collected and it is squeezed in to juice. 20 ml of this juice is pipetted in to a conical flask. It is then diluted with 25 ml of water. 2 to 3 drops of phenolphthalein is added as indicator. It is then titrated against 0.1 N of NaOH is then taken in a burette. End point is determined by the appearance of a permanent pale pink colour.

ACID-BASE TITRATON

An acid–base titration is a method of quantitative analysis for determining the concentration of an acid or base by exactly neutralizing it with a standard solution of base or acid having known concentration. A pH indicator is used to monitor the progress of the acid–base reaction.

Acid is titrated with a base and base is titrated with an acid. The endpoint is usually detected by adding an indicator. In a titration, the equivalence point is the point at which exactly the same number of moles of hydroxide ions have been added as there are moles of hydrogen ions

The two common indicators used in acid-base titration is Phenolphthalein and methyl orange. In the four types of acid-base titrations, the base is being added to the acid in each case.

EXPERIMENT

Here we adopted method 3 to find the oxalic acid content in bilimbi. Bilimbi was collected from coastal area of Kerala. Two types of bilimbi were taken for experiment. Ripen and half ripen forms of bilimbi. Both of them are crushed at first.

Ripened Half ripened

45ml of juice is obtained from 66.107g of ripen bilimbi. From this, weight of bilimbi needed for 20 ml juice is calculated. Approximately 0.4 g anhydrous sodium hydroxide is made up to 100 ml to obtain 0.1N NaOH and is filled in a burette. 20ml of extract is pipetted to a conical flask and diluted with 25 ml water.

2-3 drops of phenolphthalein is added to this as indicator. This solution is titrated against 0.1N NaOH taken in the burette.

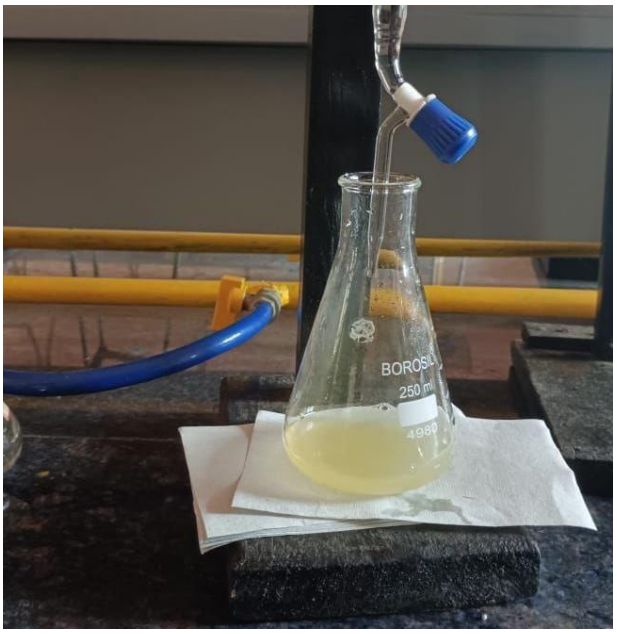
End point is determined by noting the colour change into permanent pale pink colour.

Before

After

The same experiment is repeated with half ripen bilimbi. 63.5 ml of juice is obtained from 100.154 g of half ripen bilimbi. From this, weight of bilimbi needed for 20 ml juice is calculated. Approximately 0.4 g anhydrous sodium hydroxide is made up to 100 ml to obtain 0.1 N NaOH and is filled in a burette .20 ml of extract is pipetted to a conical flask and diluted with 25 ml water.2-3 drops of phenolphthalein is added to this as indicator. This solution is titrated against 0.1 N NaOH taken in the burette.

End point is determined by noting the colour change into permanent pale pink colour.



RESULTS AND DISCUSSION

For Ripened fruit

Normality of NaOH = weight in grams/(equivalent weight x volume in litre)

$= 0.412/ (40 \times 0.1) = 0.103$ N

$N_{(NaOH)} \times V_{(NaOH)} = N_{(oxalic\ acid)} \times V_{(oxalic\ acid)}$

$N_{(oxalic\ acid)} = N_{(NaOH)} \times V_{(NaOH)} / V_{(oxalic\ acid)}$

$= (0.103 \times 28.5)/20$

$= 0.1467$ N

$W_{(oxalic\ acid)}$ = N x Eq. weight x Volume

$=0.1467 \times 63 \times 0.02$

$=0.1849$ g

20 ml of the extract contains 0.1849 g of oxalic acid

45ml of extract was obtained from 66.107 g of Bilimbi; Hence, to obtain 20 ml of extract = (66.107 X 20)/45= 29 g of Bilimbi should be taken

Therefore 29 g of Bilimbi contains 0.1849 g of oxalic acid.

For Half Ripened fruit-

Normality of NaOH = weight in grams/ (equivalent weight x volume in litre)

=0.410/ (40 x 0.1) = 0.1025 N

$N_{(NaOH)} \times V_{(NaOH)} = N_{(oxalic\ acid)} \times V_{(oxalic\ acid)}$

$N_{(oxalic\ acid)} = N_{(NaOH)} \times V_{(NaOH)} / V_{(oxalic\ acid)}$

= (0.1025 x 34.2)/20

= 0.1752 N

$W_{(oxalic\ acid)}$ = N x Eq. weight x Volume

=0.1752 x 63 x 0.02

=0.2208 g

20ml of the extract contains 0.2208 g of oxalic acid; 63.5 ml of extract was obtained from 100.154 g of Bilimbi

Hence, to obtain 20 ml of extract = (100.154 X 20)/63.5 = 31.5g of Bilimbi should be taken

Therefore 31.5 g of Bilimbi contains 0.2208g of oxalic acid.

100 g of bilimbi contains 0.629 g of oxalic acid and 100 g of half ripen bilimbi contains 0.7 g of oxalic acid.

CONCLUSION

Through acid base titration method, we found out the oxalic content in the bilimbi. The Bilimbi was collected from coastal regions. It was clear that the content of oxalic acid is different for different ages. And also, it can vary during different seasons.

Based on results, it may be concluded that the half ripen bilimbi (0.629 g) contains more oxalate content than ripen bilimbi (0.7 g).

However, the oxalate content when reached in our body, it can create various effects. Oxalate once consumed, can bind to minerals to form compounds, including calcium oxalate and iron oxalate. This mostly occurs in colon, but can also take place in kidneys and other parts of urinary tract. Sometimes they bind to form crystals, can lead to the formation of kidney stones and other health problems, especially when oxalate is high and urine volume is low.

Foods high in oxalate should be consumed in moderation to ensure optimum intake of minerals from the diet. High oxalate foods should be cooked to reduce the oxalate content

Some proponents of low oxalate diets say people are better off not consuming foods rich in oxalates, since they may have negative health effects.

However, it’s not that simple. Many of these foods are healthy, containing important antioxidants, fibre, and other nutrients. Therefore, it’s not a good idea for most people to completely stop eating high oxalate foods. Calcium also helps reduce the absorption of oxalate. Diets with less than 50 mg of oxalate per day can be balanced and nutritious.

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Department Christ College
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Place: Irinjalakuda
Date:27 April 2023

DECLARATION

I Hereby declare that the project work entitled "Determination of free oxalic acid content in Bilimbi fruit" is a work done by me under the guidance of Jibin A. K, Associate Professor of Chemistry, Christ College (Autonomous), Irinjalakuda and has not been included in any other thesis submitted by me for the award of any other degree.

JESLIN JOY
Reg.no: CCAUSCH041

Final Semester B.Sc. Chemistry Student

Christ College (Autonomous), Irinjalakuda

ACKNOWLEDGEMENT

I would like to begin by expressing gratitude to God Almighty for all his blessings.

With great pleasure, I express my sincere gratitude to Dr. Jibin A.K, Assistant Professor, Department of Chemistry, Christ College (Autonomous), Irinjalakuda, for his dynamic effort in guiding and instructing me for the completion of this work successfully.

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ABSTRACT

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DETERMINATION OF OXALIC ACID CONTENT IN BILIMBI FRUIT

Project work

Submitted to Christ College (Autonomous), Irinjalakuda

(University of Calicut) in partial fulfilment of the

requirements for the award of Degree of

BACHELOR OF SCIENCE IN CHEMISTRY

Submitted by

JOYCE VINCENT V

Reg.no: CCAUSCH042

RESEARCH AND POSTGRAGUATE

DEPARTMENT OF CHEMISTRY

CHRIST COLLEGE (AUTONOMOUS)

IRINJALAKUDA

CERTIFICATE

This is to certify that the project work entitled "Determination of free oxalic acid content in Bilimbi fruit" is an authentic work done by JOYCE VINCENT V (Reg.no:CCAUSCH042), final semester B.Sc. Chemistry student of this institution under my supervision in partial fulfilment of the requirements for the degree of Bachelor of Science in Chemistry of Christ College (Autonomous), Irinjalakuda (University of Calicut).

Dr. Jibin A K
Assistant Professor
Research and Postgraduate
Department Christ College
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Place: Irinjalakuda
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Dissertation submitted to the Christ College (Autonomous) in partial fulfilment of the requirement for the Degree of

BACHELOR OF SCIENCE

IN

CHEMISTRY

Submitted by

MIDHUL P V

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DECLARATION

I, MIDHUL P V (Reg.No.CCAUSCH043) do hereby declare that, this dissertation work entitled "**EVOLUTION OF ELECTRO CATALYTIC ACTIVITY FOR HER (HYDROGEN EVOLUTION REACTION)** " submitted to the University of Calicut in Partial Fulfilment of the requirement for the award of degree of Bachelor of Science was carried under the guidance of Dr. Dijo Damien, Assistant professor, PG And Research Department of Chemistry, Christ College (Autonomous), Irinjalakuda and it is a record of original project work carried out by me and it has not previously formed the basis for the award of, any degree, Diploma fellowship or other similar title of recognition by any other university or institutions.

Place: Irinjalakuda, MIDHUL P V

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This is to certify that **MIDHUL P V** (Reg. No. CCAUSCH043) has carried out a project work entitled "**EVOLUTION OF ELECTRO CATALYTIC ACTIVITY FOR HER (HYDROGEN EVOLUTION REACTION)**" is an authentic record of the research project carried out by my supervision and guidance in the P.G & Research Department of Chemistry, Christ College (Autonomous), Irinjalakuda. It is further certified that this project report has not previously formed the basis for the award of any Degree, Diploma, Fellowship or other similar title of recognition by any other university or Institutions.

Place: Irinjalakuda

Date: 28th April 2023

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The application of nanotechnology in green hydrogen fuel production has increased the possibility of substituting fossil fuels with this sustainable form of energy. Green hydrogen fuel can supply clean power for transportation, manufacturing units, and many other energy-dependent units. Nanotechnologies could deliver world-altering changes in the ways we create, transmit, store and use energy.

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WHY HYDROGEN IS BETTER THAN OTHER FUELS?

Hydrogen is the most abundant element in the Universe and despite the challenges associated with its extraction from water, is a uniquely abundant and renewable source of energy, perfect for our future zero-carbon needs for combined heat and power supplies. Hydrogen acts as an inherently clean source of energy, with no adverse environmental impact. Hydrogen provides a high-density source of energy with good energy efficiency. Hydrogen has the highest energy content of any common fuel by weight. Hydrogen technology does not generate greenhouse gas emissions as for fossil fuel sources.

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CHEMISTRY

Submitted by

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Date: 28th April 2023.

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HYDROGEN PRODUCTION

1. CONVENTIONAL METHOD: STEAM REFORMATION

- Reference: Ertl, G. Handbook of Heterogeneous Catalysis. Wiley 1997, 1

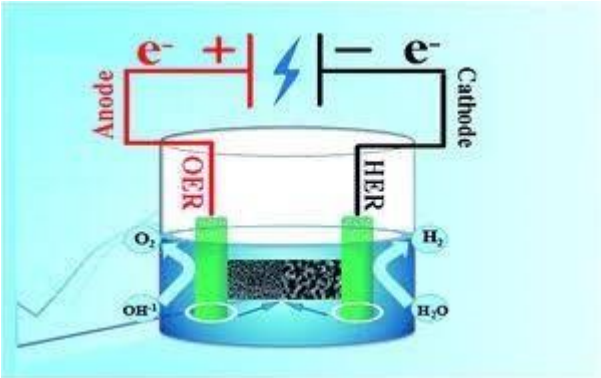
Conventionally, hydrogen is produced by the steam reformation method. This method produces hydrogen on a bulk scale and is of great commercial value.

In this method, methane reacts with steam under 1 -3 bar pressure at around 700°C–1,000°C to produce carbon monoxide and hydrogen, in the presence of the catalyst copper.

$$\mathbf{CH_4 + H_2O \leftrightarrow CO + 3H_2}$$

The hydrogen produced in this reaction is used for the synthesis of ammonia. This reaction is highly endothermic and also has a very large carbon footprint. Therefore, this cannot be considered as a convenient production method.

2. WATER SPLITTING – HYDROGEN EVOLUTION REACTION (HER)



- Reference: Sun, Y.-P.; Zhou, B.; Lin, Y.; Wang, W.; Fernando, K. A. S.; Pathak, P.; Meziani, M. J.; Harruff, B. A.; Wang, X.; Wang, H.; Luo, P. G.; Yang, H.; Kose, M. E.; Chen, B.; Veca, L. M.; Xie, S.-Y. Quantum-Sized Carbon Dots for Bright and Colorful Photoluminescence. J. Am. Chem. Soc. **2006**, *128*, *7756-7757*.

When a potential of 1.23V is applied (thermodynamic energy requirement ~236 KJ per mol), water splits to give hydrogen at cathode and oxygen at anode. Therefore, it involves two reactions namely, hydrogen evolution reaction and oxygen evolution reaction. In the present work, our focus is on the HER.

ELECTROCATALYTIC HER – MECHANISMS INVOLVED

There are two main types of HER electrocatalyst: noble-metal based electrocatalyst and non-noble metal based electrocatalyst. An electrocatalyst minimizes the energy requirement by driving the reaction through an energetically favourable kinetic pathway. The catalytic efficiency of the electrocatalyst solely relies on how the hydrogen adsorption takes place.

A simplest mechanism of HER consists of 3 steps,

- $H_3O^+ + e^- \rightarrow H_{ads} + H_2O$ **(1) (Volmer step)**
- $H_{ads} + H_3O^+ + e^- \rightarrow H_2 + H_2O$ **(2) (Heyrovsky step)**
- $H_{ads} + H_{ads} \rightarrow H_2$. **(3) (Tafel step)**

In the 1st step, hydronium ion combines with an electron to give hydrogen ads (hydrogen adsorbed on the electrocatalyst) and water. Then the hydrogen ads combine with a hydronium ion and an electron to give hydrogen and water. During the tafel step, the hydrogen ads species combine together to give hydrogen gas. The mechanism may involve either Heyrovsky step or tafel step or both, which is decided by the value of tafel's slope explained under the coming headings.

TAFEL'S EQUATION

Tafel's equation is an equation in electrochemical kinetics relating the rate of an electrochemical reaction to the overpotential**.** Tafel's equation uses certain assumptions to describe this relationship.

- The reaction at the electrode is a reaction consisting of a single electron transfer.
- The reaction at the electrode is irreversible; thus, the reverse reaction is either inexistent or negligible.
- The reaction is controlled only by an anode or cathodic process, but not both.
- The overpotential applied is very small so that it follows a linear trend with the overpotential.
- The exchange current density is constant over the potential range of interest.

The tafel's equation is given by,

$$\boldsymbol{\eta = bln(i/i_0)}$$

Where,

- **η** is the overpotential in V,
- b is the Tafel slope in V,
- i is the current density in A/m2,
- and i0 is the exchange current density in A/m2

TAFEL'S SLOPE AND SIGNIFICANCE

The term 'b' in tafel's equation is called tafel's slope. Tafel slope tells how responsive the current is to the applied voltage. A high Tafel slope shows that the bandgap energy is high which leads to a high overpotential due to the large amount of energy required to achieve activity and vice versa. Tafel slope also gives information about the rate-determining step of the electrochemical reaction. In summary, the Tafel slope explains the amount of overpotential required to achieve an activity. It helps us in knowing the role of inhibitors, the role of coatings and electrocatalyst, deeper insights like activation energy and other energy aspects Most importantly, the tafel's slope also helps us in determining the mechanism of HER, which is our present work.

If the value of b is 30 mV per dec, volmer-tafel mechanism becomes rate limiting. And if it is 40 mV per dec, volmer Heyrovsky mechanism becomes rate limiting.

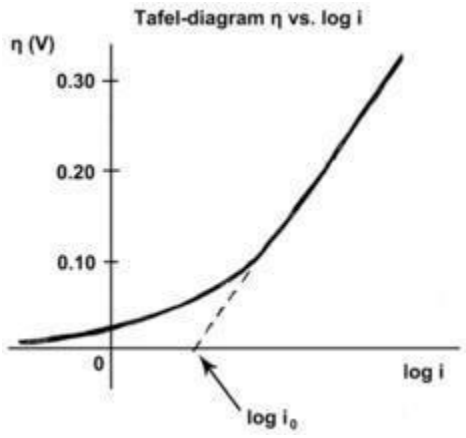


Fig. A hypothetical tafel plot

Reference: Bard, A. J.; Faulkner, L. R. "Electrochemical Methods. Fundamentals and Applications" 2nd Ed. Wiley, New York. 2001.

Here, thermoneutrality is an important factor which determines the extend of HER taking place. Should be neither too high nor too small. It must be close to zero. When $\Delta G_H >> 0$, there occurs Limited rate of adsorption of hydrogen species. When $\Delta G_H << 0$, the adsorped species find it difficult to get desrped from the surface of the electrocatalyst which leads to accumulation of hydrogen species on it. This is called catalytic poisoning.

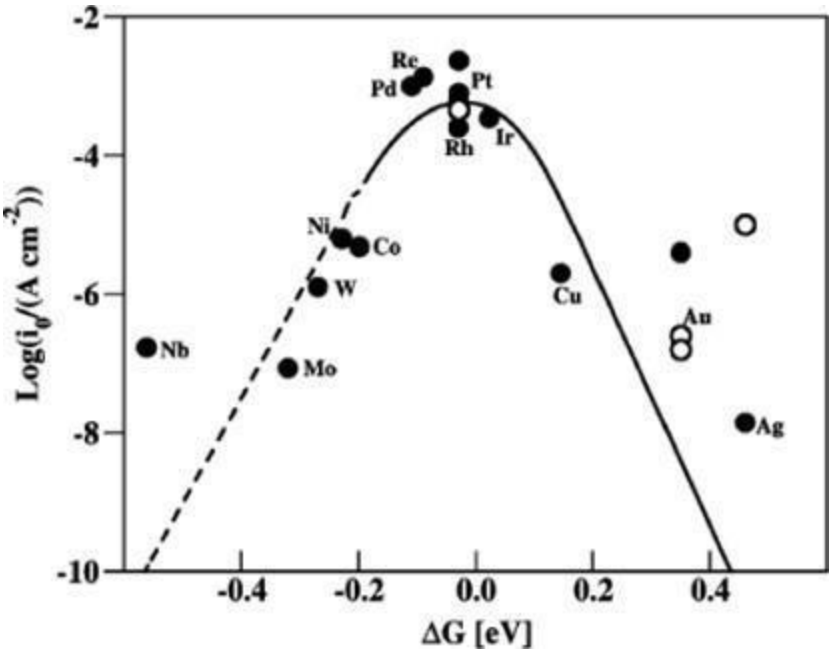


Fig. Volcano plot (current density plotted against free energy for different electrodes)

- Reference: Zhang, S. S.; Foster, D.; Wolfenstine, JProgress in energy and combustion science, 58(23):1-35, Research Gate, **2004**

A volcano curve is obtained when measured exchange currents are plotted as a function of the hydrogen adsorption free energies and a simple kinetic model is developed to understand the origin of the volcano. The volcano curve is also consistent with Pt being the most efficient electrocatalyst for hydrogen evolution

STRUCTURE OF MoS_2

The 2D structure of molybdenum disulphide bulk crystal has 2 sites on it namely, terrace site (basal plane) and edge site. For the terrace site, $\Delta G_h > 2eV$ which shows that it is not in accordance with thermo neutrality of applied potential and hence its electro catalytic activity is very low but its electrical conductivity is found to be very high. If we consider the edge site of MoS_2 bulk crystal has $\Delta G_h \sim 0eV$ implying, it has a high electro catalytic activity but its electrical conductivity is found to be very low.

For improvising the structural benefits of MoS_2 its size is reduced to in the nano size range so that its edge to basal plane ratio becomes maximized and therefore both the properties of electro catalytic activity and electrical conductivity becomes promising.

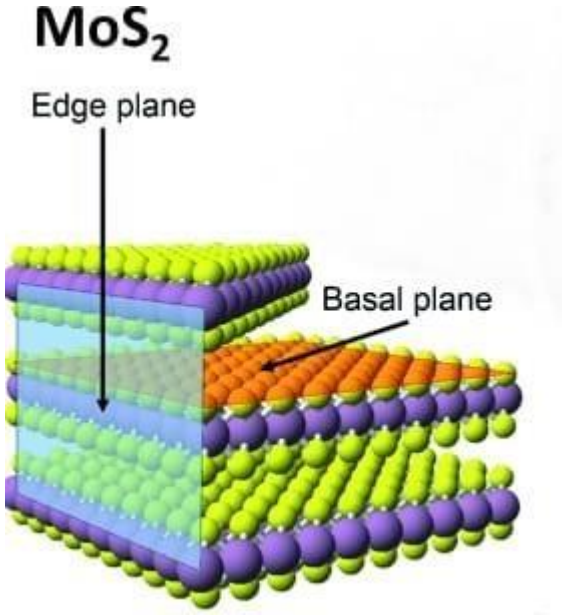


Fig: structure of MoS_2

Reference: Pristine Basal- and Edge-Plane-Oriented Molybdenite MoS_2 Exhibiting Highly Anisotropic Properties**,***Shu Min Tan, Dr. Adriano Ambrosi, Prof. Zdeněk Sofer, Štěpán Huber, Prof. David Sedmidubský, Prof. Martin Pumera*, Chemistry Europe,**2005**

MoS_2 VERSUS PLATINUM COMPARISON OF ELECTRO CATALYTIC ACTIVITY BY DETERMINING USING LINEAR VOLTAMMETRY

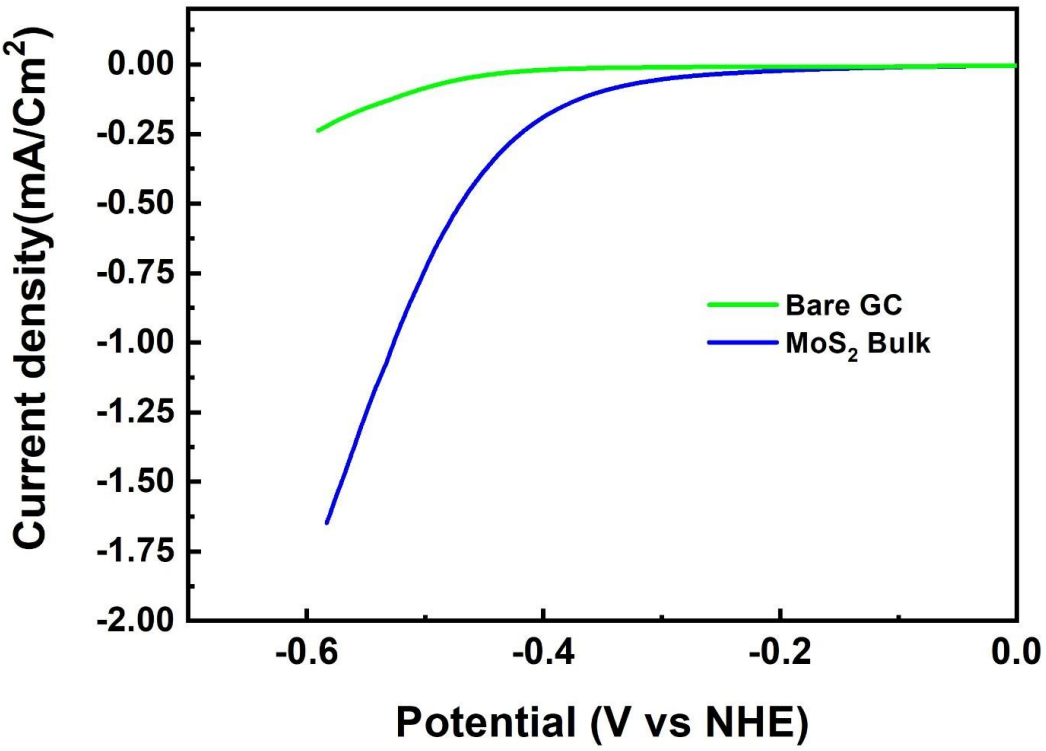
Principle- Linear sweep voltametry

Linear sweep voltammetry is a method of voltammetry where the current at a working electrode is measured while the potential between the working electrode and a reference electrode is swept linearly in time.

The plot of current vs potential is termed as linear voltammogram.

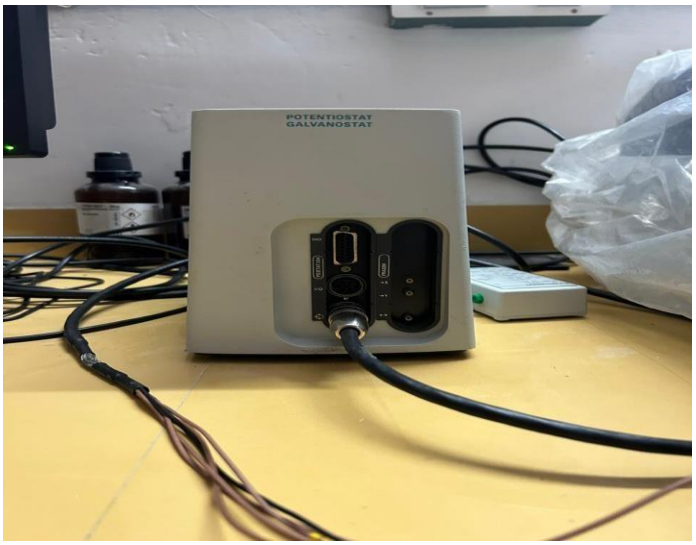
Electro catalytical activity is evaluated by plotting a linear voltammogram for MoS2

MoS_2 drop casted bare gold is taken as the working electrode, platinum as counter electrode and Ag/Agcl as reference electrode and H2So4 as electrolyte. When a potential sweep is applied current can be measured. During cathodic sweep reduction of species occur and current can be measured. During the reverse sweep there will not be much changes in current first but after reaching a particular point, reduced species undergo oxidation and the current increases giving a linear graph. The date obtained by the linear sweep of MoS2 is given below and hence the polarization curve.



We know that it is a cathodic sweep because of negative potential. When applying a potential sweep, there is no change in current first, but at a particular point reduction occurs and current increases.

INSTRUMENT USED FOR EXPERIMENT



CONCLUSION

Hydrogen is a promising fuel. Hydrogen evolution reaction plays an important role in sustainable energy development. Using Tafel's slope we can evaluate the electrocatalytic activity of a material for HER. We know that platinum is an unbeatable catalyst but due to its high cost we need to develop other material which will having the same electrocatalytic power as that of platinum and our experiment finds out that MoS2 is also a good catalyst. MoS2 in maximum edge to basal plane ratio shows maximum catalytic power so we can conclude that MoS2 can be used as a substitute catalyst in place of platinum.

REFERENCES

- Ertl, G. Handbook of Heterogeneous Catalysis. Wiley **1997**, *1*.
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RADHIKA K

ABSTRACT

The application of nanotechnology in green hydrogen fuel production has increased the possibility of substituting fossil fuels with this sustainable form of energy. Green hydrogen fuel can supply clean power for transportation, manufacturing units, and many other energy-dependent units. Nanotechnologies could deliver world-altering changes in the ways we create, transmit, store and use energy.

More efficient capture and storage of energy by use of nanotechnology may lead to decreased energy costs in the future, as preparation costs of nanomaterials becomes less expensive with more development.

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