SGT UNIVERSITY

SHREE GURU GOBIND SINGH TRICENTENARY UNIVERSITY

(UGC Approved) **Gurugram, Delhi-NCR**

Budhera, Gurugram-Badli Road, Gurugram (Haryana) – 122505 Ph. : 0124-2278183, 2278184, 2278185

Hands-On Workshop

For the students

of **Chemistry of M. Sc. And Ph. D.** on

"**Role of Molecular Docking in Drug Design: Current Perspectives**"

on 30th May 2023 by

Prof. Dr. Naidu Subbarao

Professor, Jawaharlal Nehru University (JNU) Delhi.

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Lavoisier Association,

Department of Chemistry, Faculty of Science,

ACS International Student Chapter, SGT University

organised

Hands-On Workshop

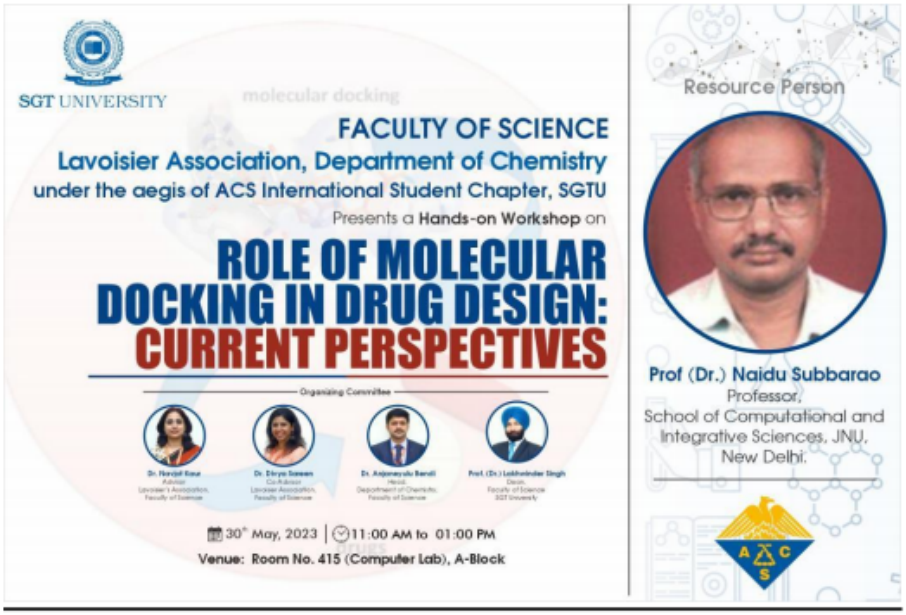
For the students

of **Chemistry of M. Sc. And Ph. D.** on

"Role of Molecular Docking in Drug Design: Current Perspectives"

on **30th May 2023**.

E-Banner



***Organizers*:** Lavoisier Association, Department of Chemistry, Faculty of Science in collaboration with the ACS International Student Chapter, SGT University.

Report of the Program:

Introduction: The hands-on workshop has been specifically arranged to impart the skills of computational technique and examination of samples for drug design. The students have been guided by Dr. Navjot Kaur (Assistant professor and Advisor at Lavoisier's Association) for the discipline and proper accomplishment of the workshop.

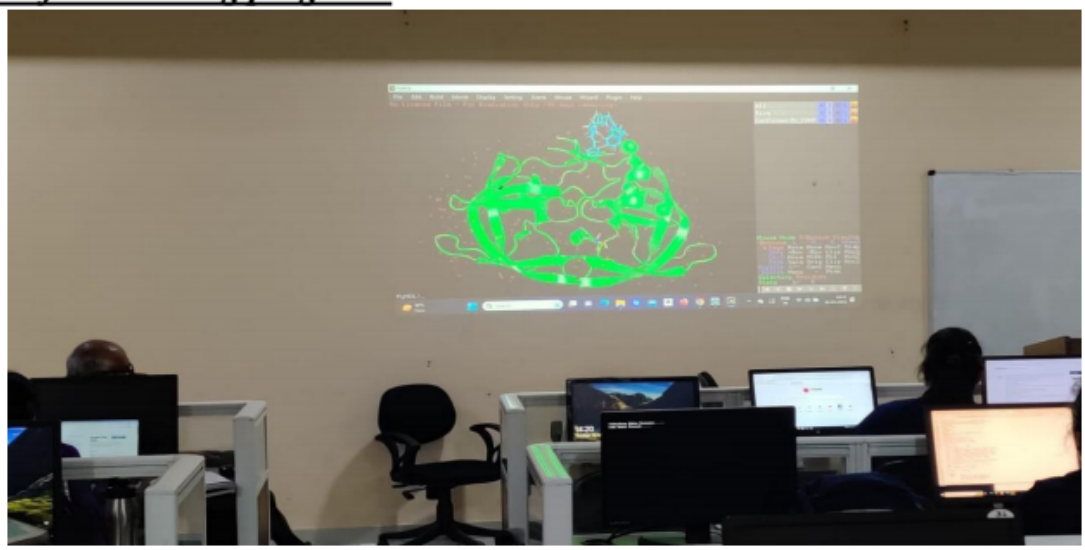
Objective of the Event: To let students understand and gain hands-on practical knowledge of drug development by computational methods.

Brief content of the event:

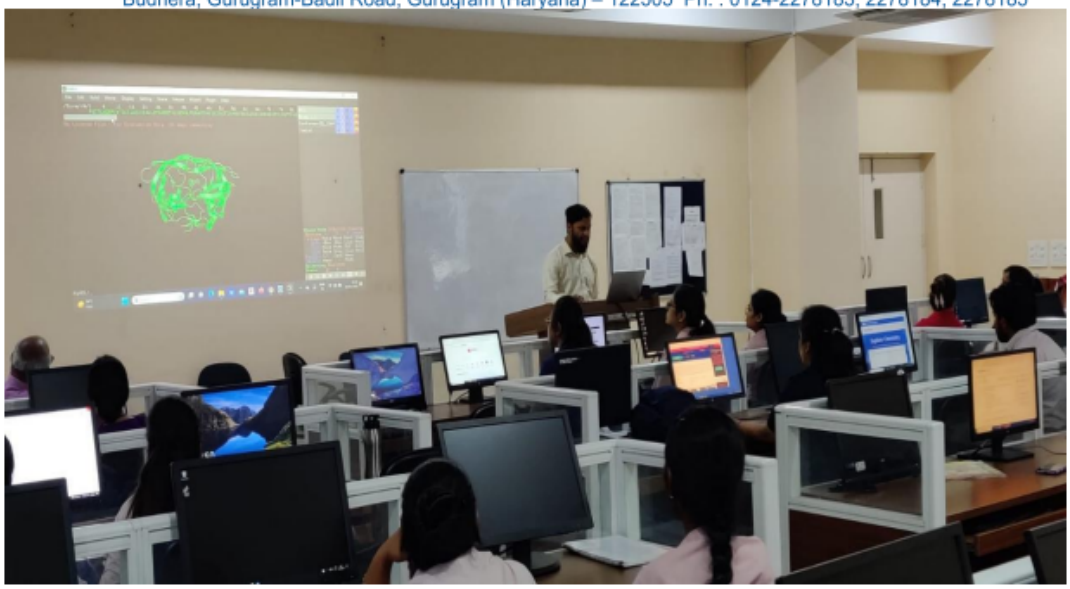
The students were first given a brief introductory talk by Prof. Dr. Lakhwinder Singh, Dean (Faculty of Science, SGT University) about the general computational and docking techniques being used in the present era. He explained the benefits of these techniques as these not only save our time and expenses but also help in saving the environment. After that, Prof. Dr. Lakhwinder Singh, Dean (Faculty of Science, SGT University), Dr. Anjaneyulu Bendi (Associate professor and HoD Faculty of Science), Dr. Navjot Kaur (Assistant professor and Advisor Lavoisier's Association), Dr. Divya Sareen (Assistant professor and Co-Advisor Lavoisier's Association) presented a sapling and token of respect and gratitude (a memento) to event's resource person. After this, the man of the event Prof. Dr. Naidu Subbarao, Professor, Jawaharlal Nehru University (JNU) Delhi started his session with the basics of Docking studies. He explained how docking addresses the interaction of drugs and receptors. The "Search and Score" method is used in docking studies. He explained that a ligand/drug should bind to only one target molecule in protein-ligand interactions. He told students about the national and international medical libraries and banks such as The Merck Manual Medical Library, Medline Plus, Health Finder, etc. Drug Target, Chemical, and IUPHAR Receptor databases were also part of the discussions. It was also found out the docking accuracy of Cerius2/PLP scoring

functions is the best among other scoring functions. The talk came to an end with the hands-on practice of docking software PYRX, PYMOL, and Auto Dock Vina. The doubts are always the interesting part of the session, and Prof. Dr. Naidu Subbarao answered every one. In the last, Dr. Divya Sareen open-heartedly thanked Prof. Dr. Naidu Subbarao for the very knowledgeable session on behalf of the whole Faculty of Science.

Glimpses of the training program:

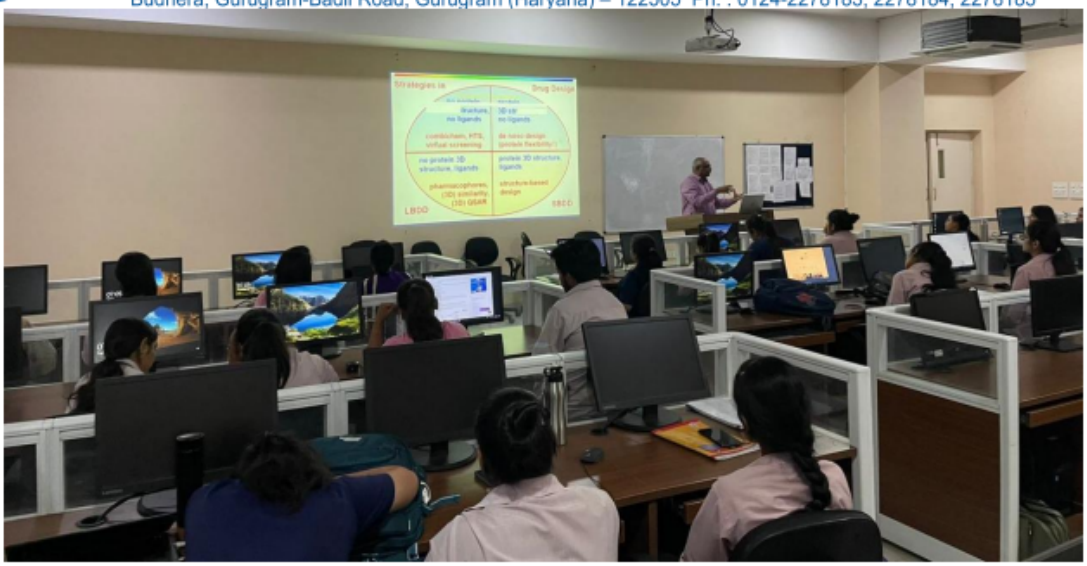


Picture 1: - Hands-on practice of ligand-protein interaction**.**



Picture 2: - Students trying their hands with the docking software.

Picture 3: - Prof. Dr. Naidu Subbarao addressing students.



Picture 4: - Prof. Dr. Naidu Subbarao interacting with students and taking their doubts.

A total of 34 students of M.Sc. Chemistry and 6 Ph.D. scholars on 30th May 2023 attended this Hands-On Workshop and got practical experience in operating Docking software and also learned the mechanism of drug design. There was an elaborate explanation and live demonstration by the expert Prof. Dr. Naidu Subbarao regarding drug design using Docking and Computational studies.

The idea of keeping the whole workshop very informative, and full of knowledge and learning came to a successful end.

Thank you.

Hands-on Workshop on Role of Molecular Docking in Drug Design: Current Prespectives

Organised by

Lavoisier Association, Department of Chemistry, under the aegis of ACS International Student Chapter, SGTU

Academic Year: 2022-2023 Date of Event: May 30, 2023

Sr. No.	Registration Number	Name of Participant	Class	Remarks
1	211706002	DEEPSHIKHA GAUR	M.Sc -2	P
2	211706003	UMESH	M.Sc -2	P
3	211706004	VIJETA CHAUHAN	M.Sc -2	P
4	211706005	BHARTI GEMINI	M.Sc -2	P
5	211706006	ISHITA GUPTA	M.Sc -2	P
6	211706007	SMRITI SHARMA	M.Sc -2	P
7	211706009	VISHAKA CHAUHAN	M.Sc -2	P
8	211706010	USHA	M.Sc -2	P
9	211706011	PINKY	M.Sc -2	P
10	211706012	SAKSHI	M.Sc -2	P
11	211706013	RASHI VERMA	M.Sc -2	P
12	211706014	NARENDER	M.Sc -2	P
13	211706015	CHINMAY	M.Sc -2	P
14	211706016	PRIYA THAKUR	M.Sc -2	P
15	211706017	RENU	M.Sc -2	P
16	211706018	MANSI	M.Sc -2	P
17	211706019	SAKSHI	M.Sc -2	P
18	211706021	DEVYANSHU	M.Sc -2	P
19	221706001	Nishi Gautam	M.Sc -1	P

	221706002	Sejal	M.Sc -1	P
22	221706003	Nidhi Sharma	M.Sc -1	P
23	221706004	Mansi Sehrawat	M.Sc -1	P
24	221706005	Shivani Yadav	M.Sc -1	P
25	221706006	Bharti	M.Sc -1	P
26	221706007	Payal	M.Sc -1	P
27	221706008	Shubhika Goyal	M.Sc -1	P
28	221706009	Yogita	M.Sc -1	P
29	221706010	Siya	M.Sc -1	P
30	221706011	Nikita Rathee	M.Sc -1	P
31	221706012	Preeti	M.Sc -1	P
32	221706013	Vinita Yadav	M.Sc -1	P
33	221706014	Poonam Yadav	M.Sc -1	Absent
34	221706015	Asma	M.Sc -1	P
35	221706016	Dolly	M.Sc -1	P
36	221706017	Jyoti Sharma	M.Sc -1	P
37	221706018	Meenal Dalal	M.Sc -1	P
38	221706019	Varsha	M.Sc -1	Absent
39	221706020	Rahul Chauhan	M.Sc -1	Absent
40	211716001	Sweety	PhD	P
41	211716002	Rajni	PhD	P
42	211716003	Taruna	PhD	P
43	201716002	Kritika	PhD	P
44	191716001	Himanshi	PhD	P
45	201716003	Priyanka	PhD	P
46	201716004	Shilpa	PhD	P
47	201716001	Jamshed	PhD	P

Navjot

Dr. Navjot Kaur.

Divya Saree

Dr. Divya Saree

To
The Registrar
SGT University, Gurugram, Haryana, 122505

Subject: Request for the approval of change of Date and Expert for the scheduled workshop.

Dear Sir,

With reference to the letter no. **SGTU/FOSC/2023/1369 Dated 22.04.2023**, the workshop on **"Role of Molecular Docking in Drug Design: Current Perspectives"** has been scheduled by the Lavoisier Association, Department of Chemistry on **29th May 2023** with the expert **Prof. Dr. Mallika Pathak, Dept. of Chemistry, Miranda House, University of Delhi**. Due to some unavoidable circumstances, she would not be able to conduct the workshop on the mentioned date. Therefore, we have identified a new expert **Prof. Dr. Naidu Subbarao, School of Computational and Integrative Sciences, Jawaharlal Nehru University, New Delhi**, and he will be available on **30th May 2023**. So kindly approve the proposed expert name and new date of the event.

Thanking you,
Yours sincerely

Name and Signature of the Proposer: 26/4/23 Dr. Nayotkaur.

Forwarded by: Kindly Consider the Proposed Expert and Event date for the Same. 26/4/23 (HOD, Dept. of Chemistry)

Dean – FOSC

Dean
Registrar, SGTU
Kindly Consider

Faculty of Science
SGT University
Budhera, Gurugram
26/4/2023

Registrar
SGT University
Budhera, Gurugram
26/5/23

29/5/23

29/5/2023

D/VC/1616
23/05/23

Faculty of Science

R-1705
23/05/23

Ref. No.: SGTU/FOSC/2023/1369

Dated: 22/05/2023

Lavoisier Association in collaboration with ACS International Student Chapter, Department of Chemistry, Faculty of Science, SGT University is proposing to organise a hands-on workshop on **"Role of Molecular Docking in Drug Design: Current Perspectives"** on 29th May 2023 from 2:00 PM – 4:00 PM.

Kindly consider and allow for the same.

Details of the event is given below:

Date: 29th May 2023 **Timings: 2:00 PM- 4:00 PM**
Venue: Room No. 415 (Computer Lab), A-Block

S. No.	Details of Resource Person	Affiliation
1	Dr. Mallika Pathak	Professor, Department of Chemistry, Miranda House, University of Delhi.

Faculty Coordinators:
Dr. Navjot Kaur, Assistant Professor, Department of Chemistry, FOSC
Dr. Divya Sareen, Assistant Professor, Department of Chemistry, FOSC

Please approve:

S. No	Requirements	Quantity	Amount (Rs)
1	Honorarium	01	4500/-
2	Memento	01	535/-
3	Sapling	01	100/-
4	e- Banner design	01	-
5	Photographer	01	-
6	High Tea & Lunch	04	160+ 1200 = 1360/-
	Total		**6495/-**

Navjot 22/5/23

Requested by: Dr. Navjot Kaur

Kindly grant the permission to organize the same
Forwarded to Dean Sir for consideration
22/5/23

Forwarded by:

Head
Department of Chemistry
Faculty of Science
SGT University, Budhera, Gurugram

Dean – FOSC

Kind Approval
The Registrar
SGT University

22/5/2023
Faculty of Science
SGT University
Budhera, Gurugram

Request may be considered for approval please

23/5/23

Dean Science

VC

Approved

Registrar
SGT University
Budhera, Gurugram
22/5/23

Registrar

24/5/23

Requisition Form

Name of the faculty: Science
Name of the department: Chemistry
Name of the coordinator & email: Dr. Nayat Kaur nayatkaur@sgtuniversity.org
Contact no. of the coordinator: 9876168143
Event title: Role of molecular Docking in Drug
Event date & time: 30/5/23 | 11.00 - 1.00 PM
Venue details: ROOM No - 415
No. of seats:

Requirement Details

A. Printing & Promotion (Tick against the requirement)

i	Design Type	Flex ☐	Banner ☑	
ii	Whether design proposal attached	Yes ☐	No ☐	
iii	Size Required			
iv	Quantity Required			

B. Photo / Video (Tick against the requirement)

i	Photography ☑	Videographer ☑	
	No. of photographers required: 01	No. of Videographers required:	

C. Vehicle Details

i	Type of vehicle	NA			
ii	No of passengers				
iii	Whether any luggage (Y/N)				
iv	Details of journey	Pick-up point:		Drop point:	
v	Time	From:		To:	
vi	Purpose of duty	Official ☐	Regular Trip ☐	Others (please specify) ☐	

D. Accommodation /Meal

Type of accommodation			Meal (Y/N)	
Duration	From		To	

E. Others

Please check the items required with respect to the above event along with quantity

	Items	Y/N	Qty	Description (if any)
i	Sapling	Y	01	
ii	Bouquet			
iii	Decoration			
iv	Projector			
v	Speakers			
vi	Screen			
vii	Mike			
viii	High Tea/Lunch	Y	04	Rs. 160 + 1200 = 1360/=
ix	Momento	Y	01	
x	Honorarium	Y	01 @ 4500/-	

Please give any additional details with respect to the above event:-

Assigning Details

Particulars	Designing	Photo/Video	Vehicle	Others
Assigned to:				
Department:				
Contact number:				

Date of submission: 22/05/2023

Signature of Dean: 22/5/2023

Registrar
SGT University
Budhera, Gurugram
24/5/23

Signature of Coordinator: Nayat

Sarvjit S Jaswal
G.M Administration
SGT University
Budhera Gurugram
25/05/2023

Assential guidelines
1) This requisition shall be raised seven days prior to the event
2) In case the even is rescheduled, postponed or cancelled, kindly intimate the concerned department immediately

Naidu Subbarao

Professor, School of Computational and Integrative Sciences,
Jawaharlal Nehru University

Molecular Modeling
Structure based Drug Design
Stuctural Bioinformatics
Cooperativity in macromolecules

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18 articles 31 articles

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TITLE	CITED BY	YEAR
Ligand binding strategies of human serum albumin: how can the cargo be utilized? A Varshney, P Sen, E Ahmad, M Rehan, N Subbarao, RH Khan Chirality: The Pharmacological, Biological, and Chemical Consequences of …	360	2010
Interaction of mitoxantrone with human serum albumin: Spectroscopic and molecular modeling studies SN Khan, B Islam, R Yennamalli, A Sultan, N Subbarao, AU Khan European Journal of Pharmaceutical Sciences 35 (5), 371-382	209	2008
Stereo-selectivity of human serum albumin to enantiomeric and isoelectronic pollutants dissected by spectroscopy, calorimetry and bioinformatics E Ahmad, G Rabbani, N Zaidi, S Singh, M Rehan, MM Khan, SK Rahman, ... Plos one 6 (11), e26186	142	2011
Elimination of endogenous toxin, creatinine from blood plasma depends on albumin conformation: site specific uremic toxicity & impaired drug binding A Varshney, M Rehan, N Subbarao, G Rabbani, RH Khan PLoS One 6 (2), e17230	118	2011
Biophysical insight into furosemide binding to human serum albumin: a study to unveil its impaired albumin binding in uremia N Zaidi, E Ahmad, M Rehan, G Rabbani, MR Ajmal, Y Zaidi, N Subbarao, ... The Journal of Physical Chemistry B 117 (9), 2595-2604	116	2013
Identification of novel target sites and an inhibitor of the dengue virus E protein R Yennamalli, N Subbarao, T Kampmann, RP McGeary, PR Young, ... Journal of computer-aided molecular design 23, 333-341	84	2009
Biophysical insight into the anti-amyloidogenic behavior of taurine SK Chaturvedi, P Alam, JM Khan, MK Siddiqui, P Kalaiarasan, ... International journal of biological macromolecules 80, 375-384	81	2015

TITLE	CITED BY	YEAR
Virtual screening, identification and in vitro testing of novel inhibitors of O-acetyl-L-serine sulfhydrylase of Entamoeba histolytica I Nagpal, I Raj, N Subbarao, S Gourinath PloS one 7 (2), e30305	75	2012
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Structural and biochemical studies of serine acetyltransferase reveal why the parasite Entamoeba histolytica cannot form a cysteine synthase complex S Kumar, I Raj, I Nagpal, N Subbarao, S Gourinath Journal of Biological Chemistry 286 (14), 12533-12541	59	2011
A robust and efficient automated docking algorithm for molecular recognition N Kasinos, GA Lilley, N Subbarao, I Haneef Protein Engineering, Design and Selection 5 (1), 69-75	52	1992
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Bacterial-induced expression of RAB18 protein in Orzya sativa salinity stress and insights into molecular interaction with GTP ligand ASSK Yachana Jha, Gaurav Sablok, Naidu Subbarao, Raja Sudhakar, M. H. U ... Journal of Molecular Recognition 27 (9), 521-527	36	2014
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In-silico modeling of a novel OXA-51 from β-lactam-resistant *Acinetobacter baumannii* and its interaction with various antibiotics V Tiwari, I Nagpal, N Subbarao, RR Moganty Journal of molecular modeling 18, 3351-3361	34	2012
Biochemical Analysis of CagE: a VirB4 Homologue of Helicobacter pylori Cag-T4SS M Shariq, N Kumar, R Kumari, A Kumar, N Subbarao, G Mukhopadhyay PlosOne 10 (11), e0142606	32	2015
Designing and synthesis of novel antimicrobial heterocyclic analogs of fatty acids A Ahmad, A Ahmad, H Varshney, A Rauf, M Rehan, N Subbarao, ... European journal of medicinal chemistry 70, 887-900	32	2013