

Center for Advanced Research and Innovation in Structural Biology (CARISB)



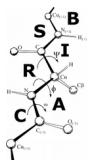
4 Day Hands-On Workshop on Molecular Docking, Virtual Screening & Computational Biology using Schrodinger Biologics Suite : A Report



By
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SCHRÖDINGER

4 Day Hands-On Workshop on Molecular Docking, Virtual Screening & Computational Biology

REPORT

ABOUT CARISB

Center for Advanced Research and Innovation in Structural Biology (CARISB) was founded in the year 2015 with a mandate to nurture, teach, train and take up research and development in advancing our current understanding about structural biology, in addition to continuing conventional activities such as drug designing, homology modeling and structure simulation studies. Currently the center is headed by Dr. Burra V L S Prasad, Professor at Amity Institute of Biotechnology, Amity University Haryana.

As per the mandate, the center organizes expert lectures, Faculty development programs, endeavours in submitting Extramural project grants and conducts seminars and workshops. As part of one of the mandates and its continuing efforts to motivate, inspire and develop enthusiasm among young students and the faculty, this year as well, CARISB has organized a 4 day hands-on Workshop on Molecular Docking, Virtual Screening and Computational Biology using Schrodinger Biologics Suite.

ABOUT SCHRODINGER LLC:

Schrödinger, LLC provides scientific software solutions and services for life sciences and materials research, as well as academic, government, and non-profit institutions around the world. It offers small-molecule drug discovery, biologics, materials science, and discovery informatics solutions; and PyMOL, a 3D molecular visualization solution. The company was founded in 1990 and is based in Portland, Oregon with operations in the United States, Europe, Japan, and India.



Schrodinger Biologics Suite is a defacto standard software suite for performing the computational tasks of a drug discovery life cycle i.e., target discovery, lead discovery, lead optimization and QSAR and ADMET analysis. It should be considered as a privilege to have a such a comprehensive computational biology software suite at AIB, AUH. With such software suites, it should be possible to publish high impact articles in the domain of drug discovery & design and also has the potential to develop and patent new candidate drug molecules for dreaded and commercially important protein targets (Diseases).

With this motivation, it was decided to have specialized workshops focusing on developing skill & expertise in using Schrodinger Suite and address research questions of social, applied, fundamental and of medical importance.

WORKSHOP OBJECTIVE:

The workshop is designed to provide the theoretical background as well as a hands-on approach to Molecular Docking, Virtual screening, Protein Modeling and simulation using Schrodinger Biologics Suite. The workshop will also cover the use of different softwares and will focus on Chem-informatics methods for lead identification and optimization.



TOPICS COVERED IN THE WORKSHOP:

- ❖ Methods and Advances in computer aided drug design
- ❖ Approaches in Target selection and refinement for docking studies
- ❖ Identification and evaluation of Binding Pocket / Active site
- ❖ Docking approaches in virtual screening and Lead identification
- ❖ Modeling the unknown proteins for docking studies
- ❖ Pharmacophore modeling and virtual screening of novel compounds
- ❖ Refinement of novel leads using ADME prediction
- ❖ Similarity and dissimilarity based methods in lead identification
- ❖ 3D-QSAR Modeling and Lead optimization
- ❖ Biologics Design and Protein engineering

Resource Person(s)	: Dr. Pritesh Bhat , Senior Application Scientist, Mr. Vinod Devaraji , Application Scientist, Schrodinger Inc, India.
Date	: 23rd - 26th January 2017
Venue	: 403, Bioinformatics Lab, A-Block, AUH
Level of Participants	: Scientists/Faculty/Research Scholars/Students
Registration Fee	: Rs. 200 for Scientists/Faculty/Research Scholars Rs. 100 for Student Participants
Chief Convener	: Prof. (Dr.) Burra V L S Prasad Center for Advanced Research & Innovation in Structural Biology (CARISB) AIB, AUH

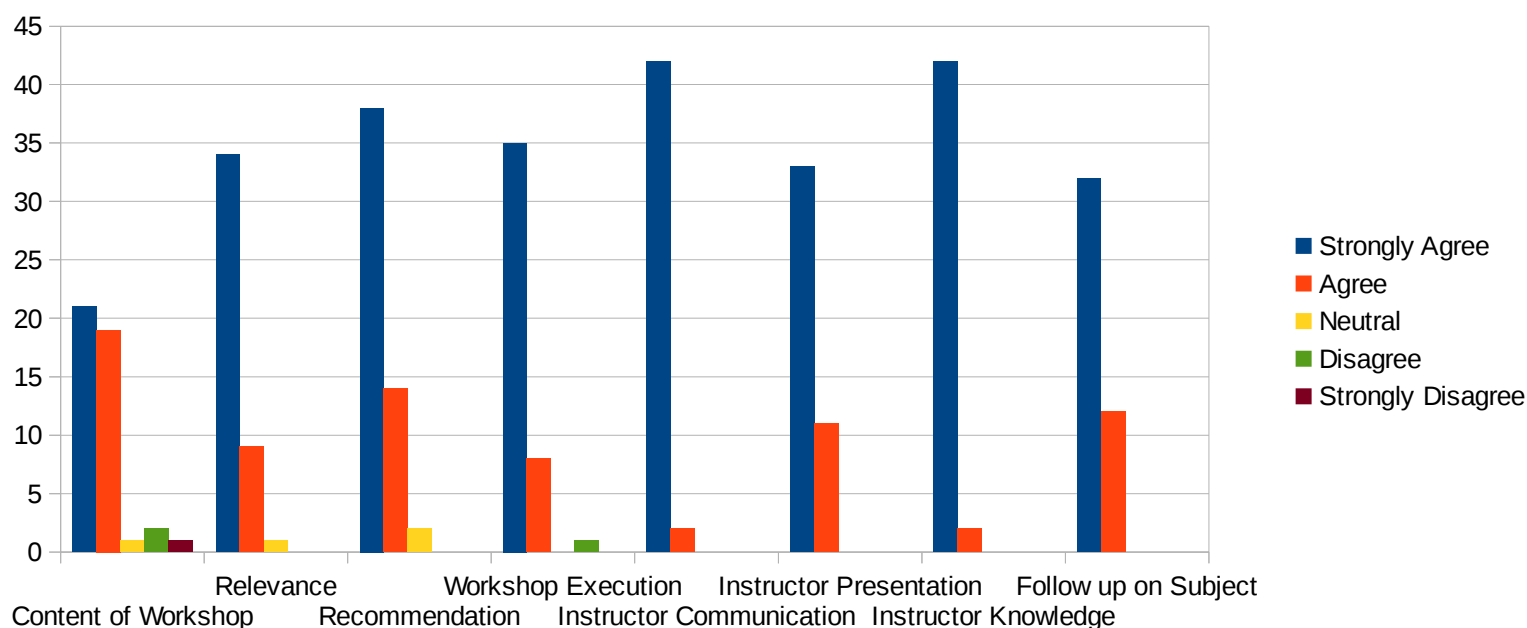
Organizing Team Members : **M.Sc. (Biotechnology) Project Students**
 Mr. Jatinder Jhaggi
 Mr. Amit Kumar
M.Tech (Biotechnology) Project Student
 Ms. Chris Gabriella Rachel..A

OBSERVATIONS AND SALIENT POINTS:

- **Overwhelming Response & Enthusiastic participation from the students, research scholars and faculty:**
 - Flyers about the workshop were circulated to relevant departments of AUH 1 month in advance followed by weekly reminders and updates.
 - The response was encouraging. The Bioinformatics Lab (403-A Block) is having only 28 PCs with another 10 workspaces having internet connection. Initially the number of participants was restricted to 35 – 40. However, considering the overwhelming response and support from the students, research scholars and faculty, the upper limit was increased to 45. The limit had to be further increased to 55 including the Organizing committee members (4).
 - We had to reject around 20 registrations because of lack of space in the Lab.
 - To accommodate the extra participants extra tables, chairs, extensions wires were arranged in the room.
 - Even on the Republic Day (National Holiday), 26th January 2017, which is the last day of the workshop, 60% of participants attended with enthusiasm.
 - **Workshop Pictures are attached at the end of the document..**
- **Certification:**
 - Mr. Dinesh Siddhu from Administration Dept., AUH designed the certificates and got them printed at ₹ 12/- per certificate.
 - The Director, AIB, Prof. Rejendra Prasad, obliged to our request and distributed certificates to all the participants.

FEEDBACK ANALYSIS:

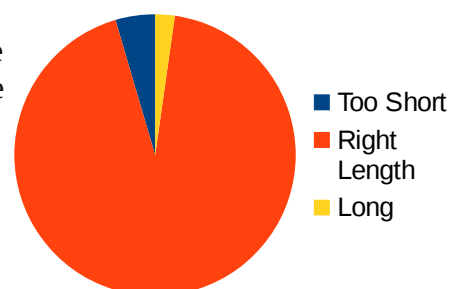
All the participants were requested to give their feed back through the feedback form .A scanned copy of the feedback form is attached at the end of the report document for reference. Around 45 participants gave their feedback. The result analysis is as follows:



The above graph reflects that > 95 % of the participants felt that the content provided, the relevance of the workshop content to the subject, the workshop implementation , the instructor's presentation and knowledge to be very good. Most of the participants have the desire to follow up the knowledge that they gained even after the workshop.

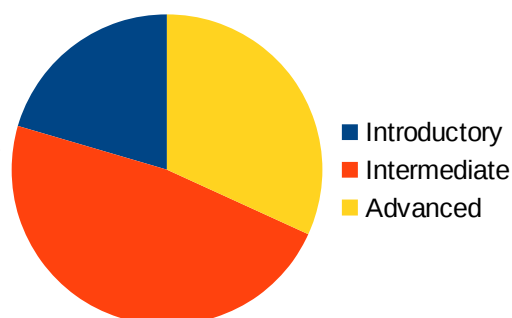
The Length of Workshop:

42 out of the 45 feedbacks received stated that the length of the workshop was optimum for the participants to get a knowledge on the subject.

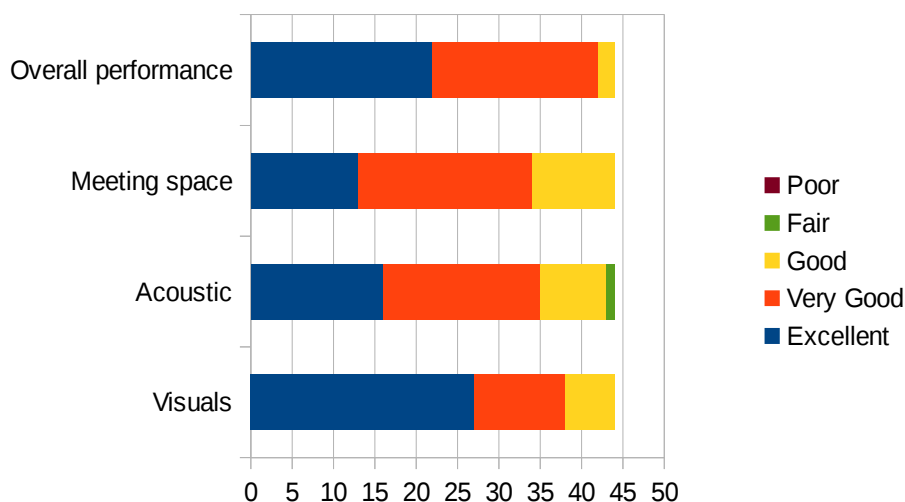


The Level of the Workshop:

Out of the 45 feed backs received, 9 felt that the level workshop is introductory, 21 felt it is intermediate and 14 felt it is advanced.



When asked about the overall performance, meeting space, acoustics and visual facilities during the workshop, > 90% have rated it to be either excellent or very good.(As shown in the graph below).



Over all the workshop feed back indicates that the participants were satisfied and it indeed was upto their expectations. It may be concluded that the objective of the workshop was achieved.

The participants would like to learn and gain expertise in Homology Modeling, QSAR, Molecular Dynamics Simulations and docking in the next 12 months.

The participants were requested for suggestions for futher improvements. A few suggestions are listed below:

- Increasing the length of the workshop
- Prior theoretical knowledge would help in understanding better.

c) Visuals should have been better. The Light shields were NOT working hence the Projected Images were NOT clearly visible.

BUDGET SUMMARY

Summary about Registration Fees

- Initially a total of 53 participants registered themselves by paying the fee. Two of the students from B.Tech-M.Tech(Dual) were absent for all the 4 days. So, we decided to give back the registration fee (₹. 200/-).
- Of the 51 registered participants, 11 were Faculty members and Research Scholars coming from AIB and ASAS of AUH. The fee collected from Faculty and Scholars: ₹. 2200/-
- 40 of the participants were students representing B.Sc. (IV sem ,VI Sem) Biotechnology, M.Tech(II Sem, IV Sem) Biotechnology, B.Tech (Bioinformatics), B.Tech-M.Tech Dual, M.Sc. Chemistry(ASAS). The fee collected from students: ₹. 4000/-
- Total fee collected : ₹. 6200/-

Summary about expenses :

- All the participants were provided Tea & Snacks twice everyday of the workshop.
- Lunch was arranged everyday for the two instructors / applications scientists who came from Schrodinger.
- The total expenses for Lunch, Tea&Snacks: ₹. 3440/-
- The Certificate Design & Printing Costs: @ Rs.12/Certificate (x 60) ₹. 720/-
- Lunch on 26th January 2017 (outside) ₹. 440/-
- Report printing ₹. 330/-
- Total expenses** ₹. 4930/-
- Cash excess after adjusting the expenses:** ₹. 1270/-

CONCLUSIONS

- Impact of the Workshop: Increased Utilization of Bioinformatics Lab resources post workshop**
 - One of the objectives of CARISB was to encourage scientific engagement and student participation in center's activities. The workshop feed back certainly shows that the objective of the center has been achieved. This is further strengthened from the observation that many research scholars, students (UG and PG) and Faculty are coming to the Bioinformatics Lab regularly during their free time and doing research on their respective topics of interest.
 - Here are a few registered users who have started using the bioinformatics lab resources for their research since completing the workshop:

S.No	Name	Designation	Project Title
1	Mr. Jatinder	M.Sc – IV Sem Student	Protein – Nucleotide second messenger interaction studies – M.Tb RecA Protein
2	Mr. Amit	M.Sc.- IV Sem Student	Protein – Nucleotide second messenger analog interactions – E.coli RecA Protein
3	Ms. Rachel	M.Tech- IV Sem Student	A bio-google search engine for Mobiles using Android Programming
4	Ms. Julie P Singh	Research Scholar	Molecular Docking studies of candidate androgen receptors
5	Ms. Shalini	Research Scholar	Homology Modeling and Docking studies on Nucleotide and Quadruplexes binding
6	Ms. Komal Yadav	B.Sc. - IV Sem Student	A study on the interaction of oestrogen – like compounds and it's hormone receptor in the human body
7	Mr. Pardeep Kumar	B.Sc. - IV Sem Student	Identification of resistant properties in White Fly

8	Dr. Sangita Venkataraman	Assoc. Professor	Protein – Protein docking studies to understand virus and plant interactions
9	Ms. Mariya	B.Tech – M.Tech Dual Student	Protein – Protein docking studies to understand virus and plant interactions
10	Mr. Shubham Mittal	B.Tech – M.Tech Dual Student	Protein – Protein docking studies to understand virus and plant interactions
11	Ms. Arti Chauhan	B.Tech – VI Sem Bioinformatics Student	Homology Modeling

- It can be concluded that the workshop is a great success and has achieved its objective of creating awareness and interest among the students, research scholars and faculty.
- CARISB is successful in achieving its objective of inspiring young minds and motivating the participants to explore the world of structural biology, target discovery and drug designing.

FUTURE PLAN OF ACTION

The success of the workshop has reinstated our confidence about the potential and opportunities of Computational Structural biology. Based on the enthusiastic participation and a positive & an encouraging feed back, given an opportunity & support, we desire to take transformational efforts through participatory initiatives and engaging-scientific activities to reach out to the fraternity to inspire, develop awareness, interest, thrill and the adventure and showcase the potential opportunities in the domain of Computational structural biology. We will organize more workshops catering to domain-specific needs and different levels of expertise. The outcome is anticipated to positively influence the admissions, quality & quantity research, teaching and training at AIB, AUH.

ACKNOWLEDGEMENT:

- We express our sincere thanks to Prof. (Dr.) P B Sharma, Hon'ble Vice Chancellor, AUH for giving the approval, instructing the necessary departments and supporting the cause.
- We sincerely express our gratitude to Sq. Ldr. S K Singh, Director, Col. Harbans Singh, Dep. Director and the members of Administration Dept who helped in arranging the additional tables, chairs, in designing the Certificate and getting them printed and also in arranging the lunch, tea & snacks for the participants.
- Our sincere thanks are due to the Col. N Dahiya, Deputy Director, Security and his team for arranging the keys for the lab which resulted in smooth functioning of the Workshop.
- Our sincere thanks to Mr. Himanshoo Bajaj, Head, IT, AUH and his IT team who took care of the Software and hardware related issues to see that the PCs and the LAN / internet are working properly.
- We sincerely express our thanks to Prof. Rajendra Prasad, Directory, AIB/ AIISH, AUH for giving the necessary support in organizing the Workshop.
- The Faculty, Research Scholars and Student fraternity are gratefully acknowledged for their enthusiastic participation throughout the workshop.
- Last but not least, we appreciate Mr. Jatinder, Mr. Amit and Ms. Rachel (coordinating team) for helping in the logistics of organising the workshop that includes coordinating with participants, instructors, report writing, seating arrangements and software installations and others.

APPENDIX

4 days Hands-on workshop on "Molecular Docking, Virtual screening and computational biology"

S.No.	Name	23rd Jan	24th Jan	25th Jan	26th Jan
1	Dr. Anil Kumar	Present	Present	Present	Present
2	Dr. Sangita	Present	Present	Present	Present
3	Dr. Munindra Ruwali	Present	Present	Present	Present
4	Dr. Seema Pathak	Present	Present	Present	Present
5	Dr. Sumittha Das	Present	Present	Present	Present
6	Dr. Ravindra Sharma	Present	Present	Present	Present
7	Dr. Debasree Ghosh	Present	Present	Present	Present
8	Dr. Kumar Garav	Present	Present	Present	Present
9	Julie Pratibha Singh	Present	Present	Present	Present
10	Shalini Aggarwal	Present	Present	Present	Present

11. Savana Musafar. (tinain786@gmail.com)

23/01/17 24/01/17 25/01/17 26/01/17

Fig :1.1 - Scanned copy of the attendance sheet of faculty participants

4 days Hands-on workshop on "Molecular Docking, Virtual screening and computational biology"

S.No.	Name	23rd Jan	24th Jan	25th Jan	26th Jan
1	Megha Sharma	Present	Present	Present	Present
2	Vaishali Rana	Present	Present	Present	Present
3	Akhila	Present	Present	Present	Present
4	Eshaa Bhardwaj	Present	Present	Present	Present
5	Monika Sohlot	Present	Present	Present	Present
6	Ritu Yadav	Present	Present	Present	Present
7	Ruchi	Present	Present	Present	Present
8	Komal Chauhan	Present	Present	Present	Present
9	Mansi Bansal	Present	Present	Present	Present
10	Daniela Gonzalez	Present	Present	Present	Present
11	Makemga Wetu Alex	Present	Present	Present	Present
12	Shashank Saxena	Present	Present	Present	Present
13	Jayesh Sanwalodia	Present	Present	Present	Present
14	Bhavya Yadav	Present	Present	Present	Present
15	Anushya Kumar	Present	Present	Present	Present
16	Muskan Yadav	Present	Present	Present	Present
17	Sacini Beniwal	Present	Present	Present	Present
18	Vansha Bhandari	Present	Present	Present	Present
19	Hitesh Hans	Present	Present	Present	Present
20	Poonam Goyal	Present	Present	Present	Present
21	Rekha Sharma	Present	Present	Present	Present
22	Kanchita Tewari	Present	Present	Present	Present
23	Pradeep Kumar	Present	Present	Present	Present
24	Tenny Thomas	Present	Present	Present	Present
25	Shubham Mittal	Present	Present	Present	Present
26	Mariya Rashid	Present	Present	Present	Present
27	Mukesh Kumar	Present	Present	Present	Present
28	Sumit Singh	Present	Present	Present	Present
29	Arti Chauhan	Present	Present	Present	Present
30	Neha Sharma	Present	Present	Present	Present
31	Anuja Yadav	Present	Present	Present	Present
32	Priyanka	Present	Present	Present	Present
33	Devashish	Present	Present	Present	Present
34	Siddhi Thapliyal	Present	Present	Present	Present
35	Gurpreet Kaur	Present	Present	Present	Present
36	Jaivinder Jhaui	Present	Present	Present	Present
37	Amit Kumar	Present	Present	Present	Present
38	Komal Yadav	Present	Present	Present	Present
39	Anshu Singh	Present	Present	Present	Present
40	Ritu Bajwa	Present	Present	Present	Present
41	Anish Yadav	Present	Present	Present	Present
42	Chris Gabriella Rachel A	Present	Present	Present	Present

Day 1/ Nikita Jaisi
Day 2/ Priyanka Yadav

23/01/17 24/01/17 25/01/17 26/01/17

Fig : 1.2 – Scanned copy of the attendance sheet of the student participants

Sanskriti Caterers
Near Power House, Manesar, Distt. Gurgaon (H.R.)
E-mail : sanskriticaterers55@gmail.com
Mobile : 9811903479

INVOICE

To, 14/3, Arindya University,
Panaggar,
Manesar.

INVOICE NO. : 1454
DATE : 30.1.2017.

Sl. No.	Description	Quantity	Rate	Amount
1	LUNCH	06	80 = 10	480 = 10
2	Biscuit (twice)	56	10 = 10	560 = 10
3	Tea (twice)	300	8 = 10	2400 = 10
				3440 = 10
Total				3440 = 10
R/off				~
TOTAL				3440 = 10

Rs/- Three thousand four hundred forty only

For Sanskriti Caterers
Authorized Signatory

PAN NO. ABTPV0454D SERVICE TAX REGN. ABTPV0454DST001

A/B - Dr. Bhanu Prasad - workshop
from 23rd to 26th January 17.
(4 days).

Fig : 2.1– Scanned copy of catering bill

Cash/Credit Memo
Bought of /Bilva

Sold to /अर्पित Sach
No./संख्या 24/11/17
Date/दिनांक 24/11/17

Qty	Description	Rate	Amount
12/1	Certificate A-4 Size	720/-	

For workshop of Prof. Burra
Molecular Docking, Virtual Screening
& Computational Biology using Schrodinger
Biologics Suite.

Signature: [Signature]
24/11/17

Thangapal VLS Prasad
E.O.E. Total 720/-

DELTA Goods once sold will not be taken back.

CASH MEMO
नकद पत्र

Sold To /अर्पित KULFI DELHI-6
A-Royal Sweet
No. 300 Old Rao Hotel (Kapurthala)
Date/दिनांक 26/11/17

QTY	PARTICULARS	RATE	AMOUNT
215	KULFI	40.80	

TOTAL 80

Signature: [Signature]

DELTA Goods once sold will not be taken back.

Bought of /Bilva

Sold To /अर्पित Old Rao Hotel (Kapurthala)
Date/दिनांक 26/11/17

QTY	PARTICULARS	RATE	AMOUNT
9	masala dosa	90	360

TOTAL 360

Signature: [Signature]

DELTA Goods once sold will not be taken back.

Fig : 2.2- Scanned copy of bill for certifiacte printing-

Bought of /Bilva

BILL FORM
उधार पत्रिका

No. क्रमांक 9/2/2017
Date दिनांक 9/2/2017

Sold To : Amity University
MESSRS Manesar
सर्वोत्तम Chandani, Burra sir

QTY. संख्या	PARTICULARS विवरण	RATE दर	AMOUNT रकम
1-	Calender Out -		2802
2-	Spine Binding -		50

Signature: [Signature]

संख्या

Thank You !
धन्यवाद !

E.&O.E.
कृपया-पूर्व सेरी १६६

TOTAL
कुल रकम 3302.00

Signature: [Signature]

Goods once sold will not be taken back.
Interest @ 18% P.A. will be charged if it is not paid on presentation.

Fig : 2.3 – Scanned copy of bill for report printing

AMITY UNIVERSITY
GURGAON

SCHRÖDINGER

CENTER FOR ADVANCED RESEARCH & INNOVATION IN STRUCTURAL BIOLOGY
&
SCHRODINGER INC, USA

CERTIFICATE OF PARTICIPATION

This is to certify that Dr. /Mr. /Ms. BURRA VLS PRASAD participated in the 4 Day Hands-On Workshop on **Molecular Docking, Virtual Screening & Computational Biology using Schrodinger Biologics Suite**, organized at Amity University Haryana, Manesar Campus, from **January 23 – 26, 2017**

Signature: [Signature]
Prof. (Dr.) Burra V L S Prasad
Chief Convener - CARISB, AIB
Amity University Gurgaon

Signature: [Signature]
Prof. (Dr.) Rajendra Prasad
Director - Amity Institute of Biotechnology
Amity University Gurgaon

Signature: [Signature]
Prof. (Dr.) P. B. Sharma
Vice Chancellor
Amity University Gurgaon

Fig .3 – Scanned copy of the certificate template

Tulsi Pratihar Singh

Workshop Feedback Form

Your feedback is critical for CARISB, AIB to ensure we are meeting the educational needs and promises made. We would appreciate if you could take a few minutes to share your opinions with us so we can serve you better.

Please return this form to the instructor or organizer at the end of the workshop. Thank you.

Workshop title: **MOLECULAR DOCKING, VIRTUAL SCREENING & COMPUTATIONAL BIOLOGY USING SCHRODINGER BIOLOGICS SUITE**

Date: 23-26th Jan 2017

Instructor: Dr. Pritesh Bhat, Schrodinger Inc, USA

	Strongly agree	1	2	3	4	5	Strongly disagree
1. The content was as described in publicity materials							
2. The workshop was applicable to interests							
3. I will recommend this workshop to others							
4. The program was well paced within the allotted time							
The instructor was a good communicator							
6. The material was presented in an organized manner							
7. The instructor was knowledgeable on the topic							
8. I would be interested in attending a follow-up, more advanced workshop on this same subject							
9. Given the topic, was this workshop:							
10. In your opinion, was this workshop:							
11. Please rate the following:							
a. Visuals							
b. Acoustics							
c. Meeting space							
d. The program overall							
12. Any suggestions for improvement?							
13. Please describe the top two topics you would like to learn more about in the next 12 months:							

Topic 1: Molecular Docking to design drugs

Topic 2: Structure analysis including pharmacophore & H-bonding

Thank you!

Please return this form to the instructor or coordinator at the end of the workshop.

*Vaishali Rana
B.Sc (H) BT 4th sem*

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d. The program overall							
12. Any suggestions for improvement?							
13. Please describe the top two topics you would like to learn more about in the next 12 months:							

Topic 1: Molecular Docking

Topic 2: Structure Based Drug Design

Thank you!

Please return this form to the instructor or coordinator at the end of the workshop.

Dr. Singh V.

Workshop Feedback Form

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11. Please rate the following:							
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b. Acoustics							
c. Meeting space							
d. The program overall							
12. Any suggestions for improvement?							
13. Please describe the top two topics you would like to learn more about in the next 12 months:							

Topic 1: MD

Topic 2: SSA

Thank you!

Please return this form to the instructor or coordinator at the end of the workshop.

*Acti
Btech Bio-Informatics
(6th sem)
9741843529/868305486*

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11. Please rate the following:							
a. Visuals							
b. Acoustics							
c. Meeting space							
d. The program overall							
12. Any suggestions for improvement?							
13. Please describe the top two topics you would like to learn more about in the next 12 months:							

Topic 1: Pharmacophore modelling

Topic 2: Pharmacophore modelling

Thank you!

Please return this form to the instructor or coordinator at the end of the workshop.

Fig : 4.1, 4.2, 4.3 & 4.4 – Scanned copy of feedback forms



SCHRÖDINGER

4 Day Hands-On Workshop on Molecular Docking, Virtual Screening & Computational Biology

Workshop Objective:

The workshop is designed to provide the theoretical background as well as a hands-on approach to Molecular Docking, Virtual screening, Protein Modeling and simulation using Schrodinger Biologics Suite. The workshop will also cover the use of different softwares and will focus on Chem-informatics methods for lead identification and optimization.

Workshop Topics include:

- ❖ Methods and Advances in computer aided drug design
- ❖ Approaches in Target selection and refinement for docking studies
- ❖ Identification and evaluation of Binding Pocket / Active site
- ❖ Docking approaches in virtual screening and Lead identification
- ❖ Modeling the unknown proteins for docking studies
- ❖ Pharmacophore modeling and virtual screening of novel compounds
- ❖ Refinement of novel leads using ADME prediction
- ❖ Similarity and dissimilarity based methods in lead identification
- ❖ 3D-QSAR Modeling and Lead optimization
- ❖ Biologics Design and Protein engineering

Resource Person	:	Dr. Pritesh Bhat, Schrodinger Inc.
Date	:	23rd - 26th January 2017
Venue	:	403, Bioinformatics Lab, A-Block, AUH
Level of Participants	:	Scientists/Faculty/Research Scholars/Students
Registration Fee	:	Rs. 200 for Scientists/Faculty/Research Scholars Rs. 100 for Student Participants Total : 200x10, 100x38 – Rs. 5800/-
Number of Participants	:	48
Deadline	:	5:00PM, 20th January 2017
Coordinator	:	Dr. Burra V L S Prasad Center for Advanced Research & Innovation in Structural Biology (CARISB) AIB, AUH
Expenses	:	Rs. 5000/- (2 Lunch, Tea & Snacks for 4 Days) Rs. 720/- (Certificate Design & Printing Cost) @ Rs.12/Certificate x 60)

The registration fee collected above shall be deposited with Finance Dept, AUH and expenses be adjusted accordingly.

Temporary Arrangements: a) 3 - 4 Extension Chords for connecting Laptops by users b) 6 - 7 Extra Chairs c) Projector for Lectures/demonstrations

Fig : 5 – Workshop proposal

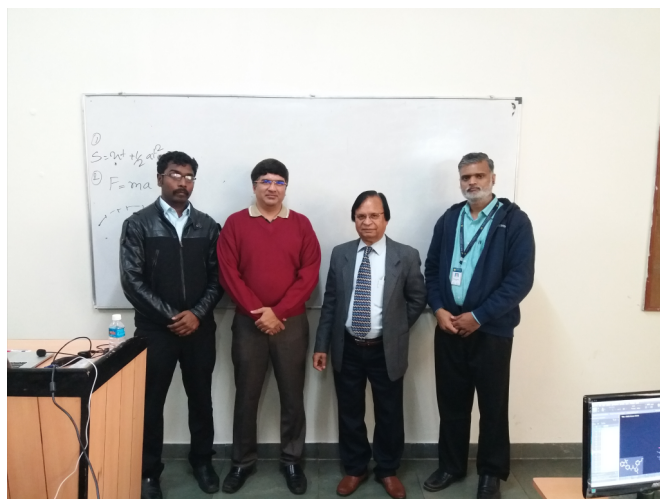
WORKSHOP GALLERY

During the Training Session



With organising committee members

With the Director (AIB)



Certificate Distribution



With the Instructors from Schrodinger

