



हिमाचल प्रदेश केंद्रीय विश्वविद्यालय
Central University of Himachal Pradesh

(Established under Central Universities Act 2009)

अस्थायी शैक्षणिक खण्ड, शाहपुर, जिला कांगड़ा, हिमाचल प्रदेश - 176206
Temporary Academic Block, Shahpur, Distt. Kangra (HP) - 176206
Website: www.cuhimachal.ac.in

File No: LS/1-5(Vol.II)/CUHP/12/173

Dated: 23.03.21

Centre for Computational Biology and Bioinformatics
School of Life Sciences

Minutes of the 8th Board of Studies meeting held on 23rd March, 2021

The meeting of the 8th Board of Studies of the Centre for Computational Biology and Bioinformatics, School of Life Sciences was held on 23rd March, 2021 by circulation (Through Online Mode).

Following Decision were taken in BOS meeting as per the Agenda.

Agenda Item-No: CBB-BOS-8/21-1: Minutes of the 7th BoS Meeting held on 29th Dec 2020. (Annexure I)

Decision:

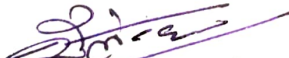
All members agreed and approved the Minutes of the 7th BoS Meeting held on 29th Dec 2020. (Annexure I).


Agenda Item-No: CBB-BOS-8/21-2: Change of the title of the PhD thesis of Smt. Neha. CUHP13RDCBB03 report attached (Annexure II)

Decision:

All members agreed and approved the change of the title of the PhD thesis of Smt. Neha. CUHP13RDCBB03 report attached (Annexure II)

The meeting ended with a vote of thanks by the chair.


Dr. Shalender Kumar Verma
Member


Dr. Sunil Kumar
VC's Nominee


Prof. Pardeep Kumar
VC's Nominee

Prof. BrijMohan
Subject Expert

Dr. Deshdeepak Singh
Subject Expert


Dr. Mahesh Kutharia
Chairman & Convenor



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PO Box: 21, Dharamshala, Himachal Pradesh-176215

Research Progress Monitoring Committee

Date: 14/10/2020

1. Name of the Candidate: Neha
2. Registration No.: CUHP13RDCCBB03
3. Date of Joining: 06/01/2014
4. Place of work: School of Life Sciences,
Central University of Himachal Pradesh
5. Members of the Research Progress Monitoring Committee:
 1. Dr. Mahesh Kulharia (Director)
 2. Dr. P. Aparoy (Supervisor)
 3. Dr. Sunil Kumar (Dean's Nominee)
6. Dates of previous Research Progress Monitoring Committee: 27/06/2018

The following to be filled by the members of the Committee

Member

- a) Has the candidate presented her/his work well? Yes
- b) Has the candidate put in enough work in the given period? Yes
- c) Do you recommend the candidate to go through the pre-Ph.D. viva (for candidates in their last Research Progress Monitoring Committee): Yes
- d) Comments of the Research Progress Monitoring Committee members on the progress of research work during the period under the report.

The work progressed well and the candidate can give Pre-Ph.D. presentation. The title of the work can be changed as proposed by the student.

Dr. Sunil Kumar
(Dean's Nominee)

Dr. P. Aparoy
(Supervisor)

Dr. Polamraasetty Aparoy

Dr. Mahesh Kulharia
(Director)



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Research Progress Committee Report- IV

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|--|---|
| 1. Name of the candidate: | Neha |
| 2. Enrolment/Registration number: | CUHPI3RDCBB03 |
| 3. School: | School of Life Sciences |
| 4. Department/Centre: | Centre for Computational Biology and Bioinformatics |
| 5. Name of the Supervisor | Dr. Polamarasetty Aparoy |
| 6. Title of Thesis: | Proposed Title: Hints for COX-2 inhibitor design: Molecular dynamics based SAR characterization and ligand based analysis. Previous Title: Application of Molecular dynamics based free energy calculation methods for identification of novel COX-2 inhibitors |
| 7. Research activities: a) Work done so far | Work done since 2018 <ul style="list-style-type: none">• Identification of novel drug like candidates against COX-2.• Structure and ligand based virtual screening using a pool of small molecule databases containing compounds of natural products, primary and secondary metabolites and FDA approved database.• A cluster of amino acids i.e., Gln178, Ser339, Tyr341, Arg499, Phe504, Val509 and Ala513 were found consistence in making interactions with different inhibitors.• MD based studies to characterize the SAR of different classes of COX-2 inhibitors.• Structural insights into the dual inhibition of COX-2/5-LOX. Work done earlier <ul style="list-style-type: none">• Ligand based Virtual Screening to identify potential dual |



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| | |
|--|--|
| b) Future plan | <p>inhibitors of COX-2 /5-LOX.</p> <ul style="list-style-type: none">• Ligand based pharmacophore modelling using CLOXIBs• Molecular descriptor profiling against COX-2 inhibitors• MD based studies to characterize the SAR of diaryl heterocyclic COX-2 inhibitors• Role of Ser516 in interactions with heterocyclic ring of COXIBs was shown.• Calculation of energetic contribution of identified amino acids• Molecular dynamics simulation based free energy calculations for COX-2 inhibitors.• Interaction based analysis of COX-2 inhibitors.• Docking studies of COX-2 inhibitors using AutoDock.• Docking of mPGES-1 inhibitors using AutoDock Vina, Dock and AutoDock.• Review of Literature. |
| | <ul style="list-style-type: none">• Pre-PhD presentation• Thesis submission• Manuscript preparation |
| <p>8. Conferences/Seminars/workshops attended and the posters, talks presented:</p> <ul style="list-style-type: none">• Poster presentation at “Accelerating Biology 2016: Decoding the deluge” held during January 19-21, 2016 organized by Bioinformatics Group, C-DAC Pune.• “International workshop on Cancer Drug Discovery and Development” held during June 22-28, 2016 at University of Hyderabad, Hyderabad.• “National Symposium on Bioinformatics & Computational Systems Biology” held during November 12-14, 2016 at Central University of Himachal Pradesh, Himachal Pradesh. | |



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9. Research work published in conference proceedings/ peer-reviewed journal:

[1] Gupta A, Chaudhary N, Kakularam KR, Pallu R, Polamarasetty A. The Augmenting Effects of Desolvation and Conformational Energy Terms on the Predictions of Docking Programs against mPGES-PLoS One. 2015;10 (8):e0134472. doi: 10.1371/journal.pone.0134472.

[2] Chaudhary N, Aparoy P. Deciphering the mechanism behind the varied binding activities of COXIBs through Molecular Dynamic Simulations, MM-PBSA binding energy calculations and per residue energy decomposition studies. J Biomol Struct Dyn. 2016 Mar 16:1-27.

[3] Gupta A, Chaudhary N, Aparoy P. MM-PBSA and per-residue decomposition energy studies on 7-Phenyl-imidazoquinolin-4(5H)-one derivatives: Identification of crucial site points at microsomal prostaglandin E synthase-1 (mPGES-1) active site. Int J Biol Macromol. 2018 Nov;119:352-359.

[4] Chaudhary N, Aparoy P. Application of per-residue energy decomposition to identify the set of amino acids critical for in silico prediction of COX-2 inhibitory activity. Heliyon. 2020 Oct; 6 (10): e04944

[5] Chaudhary N, Gupta A, Aparoy P. Molecular descriptor based profiling of COX-2 inhibitors to identify features directing COX-2 inhibition. (Under preparation)

[6] Chaudhary N, Choudhary A, Aparoy P. Development of a ligand-based pharmacophore model using PHASE and database searching: An approach for dual inhibition against COX-2 and 5-LOX. (Under preparation)

To be filled in by the candidate

1. Have you submitted your work report? Yes
2. Are there any specific problems ?
 - i. Thesis title change
 - ii. Allotment of Administrative supervisor
3. Would you like to suggest / modify any objectives: None

Date: 31-Oct-2020

Neha
Signature of the Candidate

P. Aparoy
Signature of the Supervisor

(Dr. POLAMARASETTY APAROY)

Alhami
Signature of Director of the Centre