UNIVERSITY OF JAMMU UNIVERSITY OF JAMMU RESEARCH FUND (UoJRF)

PROJECT COMPLETION REPORT

(Submit in duplicate)

- 1. Title of the project: X-ray crystallography of some organic molecules of biological relevance.
- 2. Name & Designation of Principal Investigator: Dr. Vivek Kumar Gupta Professor of Physics
- 3. Name & Designation of Co- Principal Investigator/s: -n.a.-
- 4. Duration of the project: One Year
- 5. Sanctioned grant: Rs.2,00,000/-
- 6. Date of initiation of the project: 20-01-2023
- 7. Date of closure of the project: 15-03-2024
- 8. Whether the Utilization Certificate and statement of expenditure has been submitted? Yes (If yes, mention the date and append the photocopy of the same) 07-05-2024 (copy attached)
- 9. Approved objectives:
 - To collect three-dimensional X-ray intensity data. (i)
 - To clean the data for the background associated with each reflection, the absorption that (ii) might take place due to radiation-crystal interaction, using data reduction software.
 - To process the intensity data for three-dimensional structure solution by employing (iii) various crystallographic softwares viz. SHELXS97, SHELXL97, PARST, PLATON etc.
 - To evaluate the conformational parameters (bond lengths, bond angles, torsion angles, (iv) dihedral angles etc.).
 - To calculate asymmetry parameters (ΔC_s & ΔC_2) for the determination of (v) conformations in ring molecules.
 - (vi) To determine the nature of intra- and intermolecular interactions which play a significant role when molecular packing is to be described in a unit cell.

- 10. Title of the research paper published from out of the current project work (If any, attach reprint)
 - i) "Synthesis, Crystal Structures Investigations and Hirshfeld Surface Analysis of Novel Molecule 2, 5-Dihydro [2]Benzopyrano [3,4-c] Pyrazole-water (1/4)" Chetan S. Shripanavar, Varun Sharma and Vivek Kumar Gupta Medicinal and Analytical Chemistry International Journal, Vol. 7 Issue 2 pp 1-6 (2023).
 - ii) "Crystal structure of 6-amino-3-methyl-4-phenyl-2,4-dihydropyrano [2,3-c]pyrazole-5carbonitrile" Naresh Sharma, Indrajit Karmakar, Goutam Brahmachari and Vivek Kumar Gupta

European Journal of Chemistry 15 (2) (2024) 143-148.

- 11. Title of the research paper accepted for publication from current research work (If any, attach copy of acceptance letter)
- 12. Report of the completed research project highlighting the deliverables (Attach document-Min. 3000 words) - Report attached
- 13. Details of the consumable and non-consumable (including equipment) material procured from current research project grant. - copy attached -
- 14. Has the non-consumable material (including equipment) been handed over to the concerned department? Yes/No

(If yes, attach a certificate issued by concerned HoD in this regard)

(If no, the reasons thereof) -n.a.-

15. Has the stock register carrying entries of consumable/non-consumable (including equipment) handed over to the concerned department? Yes

(If yes, attach a certificate issued by concerned HoD in this regard)

(If no, the reasons thereof)

-Certificate attached-

16. Was power point presentation of the current research work made before DRPMC by PI/Co-PI?

(If yes, attach a certificate issued by concerned Dean/ HoD in this regard)

(If no, the reasons thereof)

-Certificate attached-

The presentation was made and the work done by Prof Grupta is credible and has achieved the motivitation & objective of the project. Comments of the concerned DRPMC Members of the concerned DRPMC (Dr. Vivek Kumar Professor of Physics 4. Prof. Rakesh vaid 5. Dr. Rani Devi

UNIVERSITY OF JAMMU

POST GRADUATE DEPARTMENT OF PHYSICS

Certified that Dr. Vivek Kumar Gupta, Professor, Department of Physics, University of Jammu, Jammu has made power point presentation of the research work carried out under project no. RA/23/6033-40 dated 20-01-2023 before DRPMC on 17-5-2024 at 3.00 frm.

(Prof. Agun Bharti)

<u>Utilization of Grant released to Prof. Vivek K. Gupta (Physics Department) vide</u> <u>Research and Seed Grant Under the head Quality Assurance Fund vide No.</u> <u>RA/23/6033-40 Dated 20.01.2023.</u>

S.no	Name of the Grant	Amount of Grant Received.	Spent Grant	Balance Grant	
1.	Hiring of services /honorarium for experts	80,000/-	56050/-	23,950/-	
2.	Consumables chemicals/Glassware etc.	60,000/-	57,329/-	2,671/-	
3.	Contingency	60,000/-	45,346/-	1,4654/-	
	Grand total =	2,00,000/-	1,58,725/-	41,275/-	

Prof. Vivek K Gupta

Deputy Registrar (Grants).
University Grants

Finance Officer
University of Jammu
University of Jammu
(Finance)