**ANNEXURE-1**

**MINISTRY OF AYURVEDA, YOGA & NATUROPATHY, UNANI, SIDDHA AND HOMOEOPATHY**

**APPLICATION FOR GRANT-IN-AID**

**OF EXTRA MURAL RESEARCH PROJECTS IN AYUSH**

**Section-A**

**1.** Title of the Research Project: **Multi-Stage Screening of Medicinal Plants for Women’s Lifestyle Disorder Management *via in silico* Molecular Dynamics, Bio-Activity Guided Fractionation and *in vitro*, *in vivo* Validation**

**2.** Details of the Institution submitting the research project

Name: **University of Kalyani** Postal address: **Kalyani, District - Nadia, PIN - 741235**

**West Bengal, INDIA**

Telephone: **+913325828690**; Fax: **+913325828282**; E-mail: **registrar@klyuniv.ac.in**

Name of Collaborating Institution

Name: **The University of Burdwan** Postal address: **The University of Burdwan, Rajbati, Bardhaman, PIN -** 713104

**West Bengal, INDIA**

Telephone: **+91 9434740604** ; Fax: N/A; E-mail: **registrar@buruniv.ac.in**

**3.** In case of Individuals submitting the Research project:

(Name of the collaborating institute may be cited in S. No. 2 above)

**(i)** Name of the Principal Investigator: **Dr. Neera Sen Sarkar**

Postal address: **Department of Botany, University of Kalyani, Kalyani, Nadia**

**PIN- 741235, West Bengal, India**

Telephone: **9830545889**; Fax: -- E-mail: **neerabot19@klyuniv.ac.in**

**(ii)** Name of the Co-Principal Investigator: **Dr. Arunima Biswas**

Postal address: **Department of Zoology, University of Kalyani, Kalyani, Nadia**

**PIN- 741235, West Bengal, India**

Telephone: **9836793528**; Fax: -- E-mail: **arunima10@klyuniv.ac.in**

**(iii)** Name of the Co-Principal Investigator: **Dr. Analabha Roy**

Postal address: **Department of Physics, The University of Burdwan,**

**PIN- 713104, West Bengal, India**

Telephone: 9903843109 ; Fax: N/A E-mail: **aroy@phys.buruniv.ac.in**

**(iv)** Name of the Advisor: Prof. Prasanta Kumar Sarkar

Postal address: **Department of Rasashastra, J. B. Roy State Ayurvedic Medical College & Hospital, 170-172, Raja Dinendra Street, Kolkata- 700004, West Bengal**

Telephone: **8697970129**; E-mail: **prasantaksarkar@yahoo.com**

**4.** Name and Designation of

Principal Investigator: **Dr. Neera Sen Sarkar, Associate Professor**

Co-Principal Investigator-1: **Dr. Arunima Biswas, Assistant Professor**

Co-Principal Investigator-2: **Dr. Analabha Roy, Assistant Professor**

**5.** Duration of Research Project: **3 Years (36 months)**

The project will be executed over three years, with certain activities overlapping to ensure efficient use of time and resources. Work will be structured into half-year phases for clear milestone tracking.

**i)** Period required for pre-trial preparations: **18 months from project inception**

**Activities: Literature review, molecular docking, molecular dynamics simulation, methodology finalization, procurement, ethical/statutory clearances.**

**ii)** Period which may be needed for collecting the data: **18 months, beginning from the 6th month of inception**

**Activities: Extraction, bioassay screening, fractionation, compound isolation, and *in vivo* animal model testing.**

**iii)** Period that may be required for analyzing the data: **18 months, running in parallel with other activities, especially in the second halves of each year**

**Activities:** Statistical analysis, interpretation, and documentation of findings.

**Phase-wise Timeline of the Study:**

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Phase** | **Activity** | **Duration** | | | | | |
| **1st Year** | | **2nd Year** | | **3rd Year** | |
| **1st half** | **2nd half** | **1st half** | **2nd half** | **1st half** | **2nd half** |
| Phase 1 | Literature review, molecular docking, Molecular dynamics simulation |  |  |  |  |  |  |
| Phase 2 | Extraction & bioassay screening |  |  |  |  |  |  |
| Phase 3 | Fractionation & compound isolation |  |  |  |  |  |  |
| Phase 4 | *In vivo* animal model testing |  |  |  |  |  |  |
| Phase 5 | Data analysis & documentation |  |  |  |  |  |  |

**6.** Amount of Grant-in-aid asked for (INR):

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | **Total** | 1st Installment | 2nd Installment | 3rd Installment | Remaining Amount (10%) | Withheld Amount (10%) |
| Salary | **21,40,440/-** | **7,01,280/-** | **7,13,280/-** | **7,25,880/-** |  |  |
| Equipment | **24,00,000/-** | 24,00,000/- | -- | -- |  |  |
| Books | **--** | -- | -- | -- |  |  |
| Other Non-Recurring Expenditure | **--** | -- | -- | -- |  |  |
| Recurring Expenditure | **14,00,000/-** | 6,00,000/- | 5,00,000/- | 3,00,000/- |  |  |
| TA/DA | **1,50,000/-** | 50,000/- | 50,000/- | 50,000/- |  |  |
| Institutional Support | **2,19,000/-** |  |  |  | **2,19,000/-** |  |
| Fee of PI & CoI | **--** | -- | -- | -- |  |  |
| Misc. expenses | **6,90,000/-** | 2,30,000/- | 2,30,000/- | 2,30,000/- |  |  |
| Total | **69,99,440/-** | **39,81,280/-** | **14,93,280/-** | **13,05,880/-** | **2,19,000/-** |  |

***Detailed Estimate of Above Budget Estimate (INR)***

**Ai. Salary**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Sl. No.** | **Position**  **(2 Positions)** | **Monthly Consolidated Emolument #** | **Year 1**  **1st Installment** | **Year 2**  **2nd Installment** | **Year 3**  **3rd Installment** | **Total** |
| 1 | **Junior Research Fellow (1)** | @ 31,000/month +HRA @24% | 4,61,280/- | 4,61,280/- | 4,61,280/- | **13,83,840/-** |
| 2 | **Data Entry Operator/ Data Management Associate** | @ 20,000/month +5% annual increment | 2,40,000/- | 2,52,000/- | 2,64,600/- | **7,56,600/-** |
| **Sub-total of Ai** | | | **7,01,280/-** | **7,13,280/-** | **7,25,880/-** | **21,40,040/-** |

**Aii. Equipment**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Sl. No.** | **Equipment Name (No. of units required)** | **Unit Price** | **Year 1 1st instalment** | **Total** |
| 1 | **Software & Docking Resources (1 HPC setup)** | **24,00,000/-** | **24,00,000/-** | **24,00,000/-** |

**Aiii. Recurring (Consumables) + TA + Misc. Expenses (Analytical charges & Report Prep. etc.)**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Sl. No.** | **Recurring Expenditure Heads + Other Expenses** | **Year 1**  **1st Installment** | **Year 2**  **2nd Installment** | **Year 3**  **3rd Installment** | **Total** |
| 1 | **Consumables** | 6,00,000/- | 5,00,000/- | 3,00,000/- | **14,00,000/-** |
| 2 | **TA** | 50,000/- | 50,000/- | 50,000/- | **1,50,000/-** |
| 3 | **Misc. Exp. (outsourced analytical charge + Report prep. etc.)** | 2,30,000/- | 2,30,000/- | 2,30,000/- | **6,90,000/-** |
| **Sub-total of Aiii** | | **8,80,000/-** | **7,80,000/-** | **5,80,000/-** | **22,40,000/-** |
| **Sub-total of Ai +Aii + Aiii** | | **39,81,280** | **14,93,280/-** | **13,05,880/-** | **67,80,440/-** |

**Aiv. Institutional Support: 5% of Total Budget except Instruments = Rs. 2,19,000/-**

**Total Project Cost: Sub-total Ai+Aii+Aiii+Aiv = = Rs. 69,99,940/-**

**Justification for manpower:**

The work has several attributes which will require skilled research personal. We need a JRF who will work on the molecular docking and molecular dynamics simulation, on performing the *in vitro* assays (in 1st and 2nd year) and developing *in vivo* models by the end of 2nd year and in 3rd year. The work of the JRF is expected to generate a Ph.D after the culmination of the project.

**Justification for purchase of dedicated HPC system under equipment head:**

Kalyani University Herbal Garden is a treasure trove of biodiversity, offering a unique opportunity to explore the potential of medicinal plants in treating Polycystic Ovary Syndrome (PCOS) and related women health disorders. Our project aims to systematically screen selected plants using advanced computational methods, such as molecular docking and dynamics simulations, to predict the interactions between plant-derived compounds and key biological targets associated with these disorders.

However, the success of this project hinges on the availability of dedicated high-performance computing (HPC) resources. With a strict 3-year timeline, our project faces a significant hurdle in completing the necessary simulations within the given time frame. To overcome this challenge, we require a dedicated HPC system that can operate continuously without interruption.

The combination of advanced HPC hardware and powerful molecular dynamics software tools, such as GROMACS, will enable us to conduct detailed simulations spanning e tended time periods (up to 500 nanoseconds of simulation time). This will allow us to effectively study the kinetics and energetics of biochemical interactions between the molecules, which is crucial for identifying promising plant-derived compounds for further experimental validation. Without access to dedicated high-performance computing resources, we would be unable to perform these critical *in silico* screening and molecular dynamics studies within the 3-year project timeline. These studies form the bedrock of our research, and their successful completion is vital to the overall success of the project. Moreover, a dedicated HPC setup will not only benefit this specific project but will also serve as a valuable resource for future computational drug discovery and molecular modeling research at the University, fostering innovation and scientific advancement in the field.

**Justification for Consumables** **& Analytical Charges (to be outsourced):**

The fund will be utilized for purchasing the reagents (antibodies, assay kits for apoptosis, ROS generation, lipid profile, etc.) which are absolutely required for the proposed project. New cell lines like pancreatic cell-lines, HIT/ MIN6/INS-1/ RIN and beta-TC cells or L6 cell-lines will be procured. Cell culture media like DMEM, RPMI, serum and good quality plastic ware and glassware will also be required for growing and maintaining various cell lines required for the study. A few tests will require to be outsourced due to non-availability of specialized instruments like FTIR/ GC-MS with the PI & Co-PIs.

**Justification for Miscellaneous Expenditure:**

The fund approved for the purpose will be used for buying stationery in office, for conference registration, for printing and preparing projects reports.

**Justification of TA:**

The travel grant will be utilized for attending seminars, workshops and conferences to present the project work.

**7. DECLARATION AND ATTESTATION**

**Certified that:**

I/We have read the provisions, terms and conditions, mentioned in the Extra-mural Scheme along with its Annexure, Guidelines formulated by the Ministry of AYUSH and I/we shall abide by the relevant provisions contained under EMR Scheme and General Financial Rules of Govt. of India.

**Name and Signatures of the:**

**a) Principal Investigator:**

**b) Co-Investigator (1):**

**Co-Investigator (2):**

**c) Signature of the Head of the Institution:**

**Place:**

**Date:**

LIST OF DOCUMENTS TO BE ENCLOSED :( As per para 6.7.4 of the scheme and as uploaded on the website)