

EXECUTIVE SUMMARY
UNIVERSITY GRANT COMMISSION RESEARCH PROJECT
(F. NO. 42-862/2013 (SR) dated 23 March 2013)

1. Title of the project:

Computational Approach for Protein Structure Prediction using Self Organizing Genetic Algorithm

2. Name and address of the Principal Investigator:

V. Amouda, Centre for Bioinformatics, Pondicherry University

3. Name and address of the Institution:

Pondicherry University, R. Venkataramn Nagar kalapet, Puducherry 605014.

4. UGC approval letter no and date:

F. NO. 42-862/2013 (SR) dated 23 March 2013

5. Date of implementation: 23.03.2013

6. Tenure of the project: 23.03.2013 to 22.03.2016

7. Total grant allocated: Rs. 7, 26800/-

8. Total grant Received: Rs. 6, 98265

9. Final Expenditure: Rs.6, 69730

10: Objectives of project:

- To design the genetic operators of Genetic Algorithm
- To map the self-organizing map concept to automate the setting of right choice of parameter
- Incorporation of the designed self-organizing operators to develop a novel Self-Organizing Genetic Algorithm (SOGA)
 - To develop SOGA in JAVA platform to discover the interaction of genetic operators, to perform crossover and mutations in an automated way
- To implement the newly developed algorithm to solve a complex problem, protein structure prediction (SOGA – PSP)

- To predict structure and evaluate the performance efficiency by SOGA-PSP by
 - Torsion angles for predicting the structure was developed using SOGA
 - Resulted torsion angles were taken as input to the tinkers tool
 - Structure prediction was done using tinkers tool
 - The resulted structure were energy minimized using discovery studio and the structure with lowest energy was found to be the best
- To validate the results with the existing tool for PSP by comparative analysis

11. Whether objectives were achieved: Yes

12. Achievements from the project:

The efficiency of GA has been improved by setting appropriate parameter values, which we experimented and achieved by this project. The previously mentioned limitations has been eliminated by the incorporation of the most important parameter values of genetic operators are self-organized. This study focuses on the application of a novel genetic algorithm called the self-organizing genetic algorithm for PSP (SOGA-PSP), which self-configures the crossover and mutation rate during execution, thereby reducing the complexity, which in turn increased the performance efficiency. Research data and information are published as research article in scientific journals

13. Summary of the findings:

Protein structure prediction is one of the multi-faceted problems in biology, which is noteworthy to predict the function of proteins whose functions are unknown. In this project a new problem is described to predict the structure of proteins using SOGA (Self Organizing Genetic Algorithm) which is significant to predict the function of proteins. SOGA, a novel algorithm based on the concept of self-organization blended with genetic Algorithm. Torsion angles, the local structural parameters which define the backbone of protein are considered to encode the chromosome that enhances the quality of the

confirmation. Newly designed self-configured genetic operators are used to develop self-organizing genetic algorithm to assist the accurate structure prediction.

Peptides are used to gauge the validity of the proposed algorithm. As a result, the structure predicted shows clear improvements in the root mean square deviation on overlapping the native indicates the overall performance of the algorithm. In addition, the Ramachandran plot results implies that the conformations of phi-psi angles in the predicted structure are better as compared to native and also free from steric hindrances. The proposed algorithm is promising which contributes to the prediction of a native-like structure by eliminating the time constraint and effort demand. In addition, the energy of the predicted structure is minimized to a greater extent, which proves the stability of protein.

14. Contribution to the Society:

It reduce the time and cost of the protein structures prediction process through wet lab or experimental methods. A novel algorithm, SOGA implemented on PSP algorithm was proved to be better. The drawbacks of traditional approaches has been reduced

15. Whether any Ph.D Enrolled/ Produced out of the project: No

16. No. of Publications out of the Project:

1. AmoudaVenkatesan, JeyakodiGopal, ManimozhiCandavelou, SowjanyaGollapalli, KayathriKarthikeyan, Computational Approach for Protein Structure Prediction,Healthc Inform Res. Jun 2013; 19(2): 137-147.
2. AmoudaVenkatesan¹, DheebikaKuppusamy¹JeyakodiGopal¹, KameleshGasva¹, **Interface for Protein Structure Predictionusing Self-Organizing Genetic Algorithm**, Computers in Biology and Medicine. January 2015. International Journal of Applied Engineering Research 10(14):34720-34725

SIGNATURE OF THE PI

Dr. V. AMOUDA
Assistant Professor
Centre for Bioinformatics
Pondicherry University

SIGNATURE OF THE REGISTRAR

Registrar
Pondicherry University

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UNIVERSITY GRANT COMMISSION
BahadurshahJafar Marg, Delhi
PONDICHERRY UNIVERSITY
PONDICHERRY
ASSESSMENT/EVALUATION REPORT UGC MRP

A. DETAILS OF THE PROJECT

1. Title of the project	Computational Approach for Protein Structure Prediction using Self Organizing Genetic Algorithm
2. Total duration of the project	3 years
3. Project status	Completed
4. Subject	Bioinformatics
5. File Number UGC reference number & date	F. NO. 42-862/2013 (SR) dated 23 March 2013
6. Grant approval	UGC MRP

B. Evaluation report of the Expert member

1.	Name of the principal investigator	Dr. V. Amouda
2.	Designation	Assistant Professor
3.	Address , E-mail, phone	Center for Bioinformatics, Pondicherry University, Pondicherry 605014 E-mail: amouda@yahoo.com
4.	Whether work is focused on the title of the project	yes
5.	Whether original work is done	yes
6.	Whether significant contribution made the principal investigator	yes
7.	Whether proposed work have relevance to the society/ scientific community	Relevant to Scientific Community
8.	What type of contribution found in the final report theoretical/ practical. If there are theoretical contribution given by the principal investigator, whether real application are given	The contribution practical and the real application is taken to apply new approach in bioinformatics.
9.	Whether theoretical/ practical contribution and their results and finds are published	Yes
10.	Whether results and findings are significant	Yes
11.	Whether the significant publication are made by principal investigator in peer reviewed journal	Yes
12.	The number of publication made by the principal investigator in standard reputed journal	Yes
13.	Whether the contribution made by the principal investigator is sufficient	Yes, sufficient work has been done

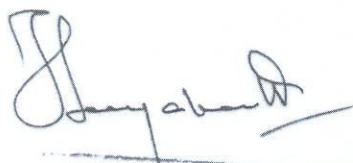
14.	The findings and results of the sanction major research projects are justifiable	yes
15.	Whether completed project work meet the proposed objective	Yes, the objective is well designed and new algorithm is developed.
16.	Give your brief comments on the overall work of the project	The development of new algorithm is automated parameter setting useful for the non –domain expert and it is novel.
17.	Any specific comments	Protein structure prediction is done by self automated algorithm, first of its kind.
18.	Indicate your overall assessment of the project poor/ good / excellent	Overall the project is very good .

Date: 27.05.2019

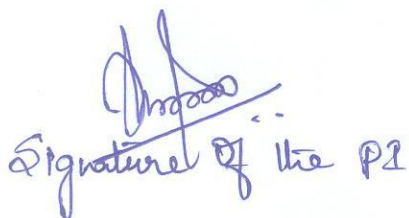
Place: Karaikudi

Name and Address of Expert:

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4.	Whether work is focused on the title of the project	yes
5.	Whether original work is done	yes
6.	Whether significant contribution made the principal investigator	yes
7.	Whether proposed work have relevance to the society/ scientific community	Relevant to Scientific Community
8.	What type of contribution found in the final report theoretical/ practical. If there are theoretical contribution given by the principal investigator, whether real application are given	The contribution by principle investigator is real application and useful for the bioinformatics.
9.	Whether theoretical/ practical contribution and their results and finds are published	yes
10.	Whether results and findings are significant	yes
11.	Whether the significant publication are made by principal investigator in peer reviewed journal	yes
12.	The number of publication made by the principal investigator in standard reputed journal	yes
13.	Whether the contribution made by the principal investigator is sufficient	Yes, sufficient

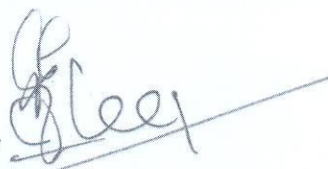
14.	The findings and results of the sanction major research projects are justifiable	yes
15.	Whether completed project work meet the proposed objective	Yes, the automated algorithm is well developed as per the objective
16.	Give your brief comments on the overall work of the project	The overall project is innovative by designing a new algorithm to MSA
17.	Any specific comments	The initiative taken for the peptide structure prediction is appreciable and good.
18.	Indicate your overall assessment of the project poor/ good / excellent	The completed project is good.

Date:
Place:
Name and Address of Expert:


27.05.2019
Bangalore

Prof. K. Sekar
Group Leader


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