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ORGANIZED BY
CSIR-CENTRAL INSTITUTE OF MEDICINAL & AROMATIC PLANTS, LUCKNOW

Training program contents:

- Introduction to Genetic algorithm (GA)
- Operators of GA
- GA-Initialisation
- GA-Fitness function
- GA-Selection
- GA-Crossover
- GA-Mutation
- GA-Survivor selection
- GA-Termination condition
- Application of GA in Molecular Docking
- Introduction to Molecular Docking
- Downloading & installation of Docking tool AutoDock/Vina
- Ligand & Receptor preparation
- File formats of AutoDock/Vina
- Molecular Docking steps
- Analyzing Docking result
- Limitation of AutoDock & Vina
- Demo exercise-AutoDock/Vina
- Practicals-AutoDock/Vina

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Dr. Feroz Khan

Coordinator
Dr. Laiq-ur Rahman

Chairman
Dr. Prabodh Kumar Trivedi
Director, CSIR-CIMAP

About CSIR-CIMAP, Lucknow

CSIR-Central Institute of Medicinal & Aromatic Plants (CSIR-CIMAP) is a premier multidisciplinary research institute of Council of Scientific & Industrial Research (CSIR), New Delhi, India with its major focus on exploiting the potential of medicinal and aromatic plants (MAPs) by cultivation, bioprospection, chemical characterization, extraction, and formulation of bioactive phytochemicals. With a strength of 100 scientists, 162 technical officers, 129 support staff and nearly 300 doctoral and post-doc scholars at its head-quarter in Lucknow and research centers at Bengaluru, Hyderabad, Pantnagar, and Purara. CSIR-CIMAP has played a key role in positioning India as a global leader in production of mints, vetiver and other aromatic grasses, and in ensuring indigenous production of artemisinin – a WHO approved antimalarial. CSIR-CIMAP houses a National Gene Bank on MAPs, which is one of the three of its kind in India. CSIR-CIMAP has played a key role in successfully commercializing an ayurvedic herbs based antidiabetic formulation, which has now benefitted millions. The institute is presently accredited by ICS-UNIDO and Indian-Ocean Rim Association (IORA) as a focal point for research and training on Medicinal Plants among 21 participating member countries. For more details please see the CSIR-CIMAP website www.cimap.res.in

About the Bioinformatics Skill Development Program

Genetic Algorithm (GA) is an adaptive heuristic search algorithm, which belongs to evolutionary algorithms. GA is based on the idea of natural selection and genetics. This algorithm is intelligent exploitation of random search provided with prior data to direct the search into the region of better performance in solution space. GA simulate the process of natural selection which means those species who can adapt to changes in their environment are able to survive and reproduce and go to next generation. In simple words, they simulate “survival of the fittest” among individual of consecutive generation for solving a problem. However, key aspects of molecular docking are (i) scoring functions, i.e., predicting the energy of a particular pose (depends on speed and accuracy), (ii) search methods i.e., finding an optimal pose, and (iii) dimensionality i.e., can we trust the answer. To solve the problem of optimal pose search, researchers used GA and the most common example is AutoDock & AutoDock Vina molecular docking softwares (free). The AutoDock-1 (1990) was the first docking method with flexible ligands, while AutoDock-3 (1998) include the free energy force field, advanced search method & AutoDockTools (ADT) graphical user interface. Current version of AutoDock is AutoDock-4 (2009), which covered number of docking parameters. More advance form version is AutoDock Vina (2009), an one step solution to docking, rewritten by Oleg Trott & Arthur J. Olson (The Scripps Research Institute, Molecular Biology, La Jolla, San Diego, CA) with new approach to scoring and search. Docking function/binding energy includes sum of dispersion/repulsion energy (ΔG_{vdw}), electrostatics energy (ΔG_{elec}) & hydrogen bonds energy (ΔG_{hbond}), desolvation energy (ΔG_{desolv}) and torsional entropy (ΔG_{tors}). AutoDock Vina scoring function is combination of knowledge-based and empirical approach. Grid maps precompute interactions for each type of atom 100 times faster than pairwise methods. Grid maps drawbacks is receptor conformationally rigid, limits the search space. In molecular docking tools two kinds of search methods are used (i) systematic and (ii) stochastic. AutoDock support following stochastic search methods e.g., simulated annealing (SA), Evolutionary algorithm method namely, Genetic Algorithm (GA), and hybrid global-local search method namely, Lamarckian GA (LGA). In the present training program we will understand the concept of GA and how a GA works, with its different operators and at last prediction of optimal ligand binding site on receptor through AutoDock tool.

The Aim of Bioinformatics Skill Development Training Program

To familiarize researchers/academicians/students with the basics & application of GA based molecular docking used in the biochemical data analysis and interpretation. Also explain the different important search parameters used in GA/Lamarckian GA e.g., Population size, Crossover rate, Mutation rate, Solis & Wets local search (LGA only) and termination criteria. Also explain the underlying principles, mathematical functions, data search algorithm with suitable easy to understand examples. In parallel, practical exercises/example demos for technical skill development will be scheduled online after introductory lectures. The training program will cover expert lectures, training program theme based/tutorial lectures, demo presentations, and online practical exercises. The training program would cover the following aspects:

- ❖ Introduction to Genetic algorithm (GA)
- ❖ Operators of GA
- ❖ GA-Initialisation
- ❖ GA-Fitness function
- ❖ GA-Selection
- ❖ GA-Crossover
- ❖ GA-Mutation
- ❖ GA-Survivor selection
- ❖ GA-Termination condition
- ❖ Application of GA in Molecular Docking
- ❖ Introduction to Molecular Docking
- ❖ Installation of AutoDock/Vina
- ❖ AutoDock file formats (Ligand PDBQT file, Receptor PDBQT file, AutoGrid parameter file (GPF) & AutoDock Parameter file (DPF))
- ❖ Molecular Docking steps in AutoDock (Run AutoGrid & AutoDock)
- ❖ Ligand & Protein/Receptor Preparation
- ❖ Analyzing AutoDock results
- ❖ When are AutoDock & Vina not suitable?
- ❖ Example demo presentation
- ❖ Practicals/Hands-on exercise

The participants may access online bioinformatics resources/literatures/reviews related to molecular docking and genetic algorithm. The online skill development training gained through this program may help in making career in structural bioinformatics, especially studying receptor-ligand interactions or binding mode conformation of proteins and inhibitors and entrepreneurship in bioinformatics/biochemical/biomedical research and development domains.

Eligibility

Graduates/PG students/Ph.D. fellows/Post-Doc scholars/ Project fellows/Technical Officers/Company Professionals/Entrepreneurs/Academicians can attend.

Certification

Training program's participants will receive a digital certificate of participation from the CSIR-CIMAP, Lucknow after successful completion of the skill development program. The digital certificate will be emailed after the successful completion of training program.

Feedback

After training program, participants may be asked to submit the given feed-back form. Participants may be asked to express their training experiences and suggestions for further improvement.

Technical requirements

Participants may have Laptop/Desktop PC with Windows 10 OS with Linux Ubuntu sub-system app, knowledge of DOS commands, Scripting knowledge on any text editor e.g., Notepad, Notepad++, and working experience of MS Office. A working version of Windows, MS Office software is necessary to follow the practical examples/training sessions online. Knowledge of basic cell biology and biostatistics will be will be beneficial.

Training mode

Online mode through MS Team or similar online app.

Registration Fee

Rs. 5,000/- (Five Thousand only) per participant. The registration fee includes digital Registration kit which includes workshop/training brochure, program schedule, tutorials, training lectures, practicals demos/exercises, feed-back form and a certificate after successful completion of training.

Registration fee can be pay through online mode to SBI bank A/c No. 00000030267691783, SBI Main branch, Hazratganj, Lucknow (IFSC code: SBIN0000125) or through Demand Draft in favor of '**Director, CIMAP**', payable to Lucknow. Complete registration form along with the fee details should reach us on or before deadline i.e., Feb. 28, 2021 upto 5:00 PM. Registration to the skill development training program will be on 'First-come-First-serve' basis. Seats are limited.

For any query related to this skill development training program, kindly contact:

Dr. Feroz Khan (f.khan@cimap.res.in)

Dr. Laiq-Ur Rahman (l.rahman@cimap.res.in).

For any further details please contact:

Director

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Registration Form

Candidate Full Name: _____

Designation/Position: _____

Affiliation (Institute/Univ.): _____

Address: _____

Locality Type (Urban/Rural): _____

Category (Gen/OBC/SC/ST): _____

Gender (Male/Female): _____

Area of Interest: _____

E-mail: _____

Contact No.: (+91) _____

Payment Details:

Registration Fee Amount: Rs. 5,000/- (Rs. Five Thousand only)

Mode of payment (Online/DD): _____

Online Transaction/DD No. _____ Date _____

Bank Name: _____

Name _____ Signature _____