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Vibin Ramakrishnan

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EDUCATION AND EMPLOYMENT

- Professor: Indian Institute of Technology, Guwahati – 781039. India (2019 -)
- Associate Professor: Indian Institute of Technology, Guwahati – 781039. India (2015-2019).
- Assistant Professor: Indian Institute of Technology, Guwahati – 781039. India (2011-2015).
- Faculty Scientist: Institute of Bioinformatics and Applied Biotechnology (IBAB) Bangalore and RGCB Thiruvananthapuram.
- Post-Doctoral Research Associate: Center for Bioinformatics, Biology, Jonsson Rowland Science Center, Rensselaer Polytechnic Institute, Troy NY – 12180, USA
- Ph.D.: Indian Institute of Technology, Bombay, Powai-400076 India
Doctoral Thesis: Stereo chemical Effects in Protein Structure Folding and De novo Design
- Master of Science: *in* Applied Chemistry. Cochin University of Science and Technology, Kochi, India. Specialization: Synthetic Polymers, Industrial Catalysis

RESEARCH INTERESTS

Bio-nanotechnology, Drug Delivery Vehicles, Network medicine, Peptide based antibiotics, Computational Biology

AWARDS & SCHOLASTIC ACHIEVEMENTS

- Innovative Young Biotechnologist Award Extension (IYBA 2011-12), Dept. of Biotechnology, Ministry of Science and Technology, Govt. of India.
- Innovative Young Biotechnologist Award (IYBA 2007-08), Dept. of Biotechnology, Ministry of Science and Technology, Govt. of India.
- Post-Doctoral Fellowship funded by National Science Foundation, United States
- Institute Research Fellowship, IIT Bombay
- CSIR-UGC Test, Graduate Aptitude Test in Engg. (GATE)
- Cochin University Merit Scholarship by CUSAT for top two students in each discipline

PROFESSIONAL AFFILIATIONS

- Member, National Academy of Sciences. India
- Member, American Chemical Society
- Member, International Society for Computational Biology (ISCB).
- Biophysical Society

MOLECULAR INFORMATICS & DESIGN LABORATORY

PI: Prof. Vibin Ramakrishnan

Dr. Vibin Ramakrishnan is a Professor of Biosciences and Bioengineering, IIT Guwahati. Dr. Vibin earned his Master's in Applied Chemistry from Cochin University of Science and Technology and Ph.D. from School of Biosciences and Bioengineering, IIT Bombay. He worked as a Postdoctoral Research Associate at Rennselaer Polytechnic Institute, New York and a Faculty scientist at IBAB Bangalore, before joining Department of Biosciences & Bioengineering at IITG. He has about 50 publications in reputed international journals and 10 patents, including an international patent to his credit. He is the principal scientific advisor of two biotech companies. The Department of Biotechnology, Govt. of India has awarded Vibin, the Innovative Young Biotechnologist Award (IYBA) in the year 2007-08 to recognize his contributions and innovative approach in biotechnology research.

PhD Students (Graduated: 8, Ongoing: 4)

No	Name	Area(s) of Research	Completed / Ongoing	Supervisor / Co-Supervisor
1	Prakash Kishore Hazam	Peptide Drugs	Defended	Supervisor
2	Arnish Chakraborty	Infectious Diseases	Defended	Co-Supervisor
3	Sajitha S.	Functional nano assemblies	Defended	Supervisor
4	Gaurav Jerath	Drug Delivery Vehicles	Defended	Supervisor
5	Gaurav Pandey	Chemical Neuroscience	Defended	Supervisor
6	Debika Datta	Biophysics Peptide Chemistry	Defended	Co-Supervisor
7	Ruchika Goyal	Drug Delivery Vehicles	Defended	Supervisor
8	Jahnu Saikia	Chemical Neuroscience	Defended	Supervisor
9	Vivek Gupta	Bionanotechnology	Defended	Supervisor
10	Yvonne Christian	Drug Delivery Vehicles	Ongoing	Supervisor
11	Kalpana Kumari	Bionanotechnology	Ongoing	Supervisor
12	Amay Sanjay Redkar	Network Medicine	Ongoing	Supervisor
13	Mouli Sarkar	Networ Medicine	Ongoing	Supervisor

M.Tech Dissertations (Graduated: 9)

No	Name	Research Area	Status	Role
1	Indrani Ray	Protein folding	Completed	Supervisor
2	Prem Prakash Das	Protein aggregation	Completed	Supervisor
3	Vinayak Suresh Pevekar	Modeling tools	Completed	Supervisor
4	Anjali Singh	Peptide drugs	Completed	Supervisor
5	Mukesh B	Bionanotechnology	Completed	Supervisor
6	Akhil R	Molecular Dynamics Simulations	Completed	Supervisor
7	Franklin P M	Peptide Drugs	Completed	Supervisor
8	Amay Sanjay Redkar	Peptide Drugs	Completed	Supervisor
9	Shreya Bhattacharya	Network Medicine	Completed	Supervisor
10	Amit Bhandari	Network Medicine	Completed	Supervisor

B.Tech Dissertations (Graduated: 10)

1. Ashwini Kumar. Profiling electrostatic interaction of protein segments involved in aggregation, self-assembly and cell penetration
2. Rakesh kumar choudhary. Virtual Activity Profiling of Drug-Target Complexes by 2D Fingerprinting.
3. Shashank Sekhar. Cellular Decision making of B.Subtilis under stressful conditions.
4. Nitin Gacche. Mutational Effects in Protein Folding Kinetics
5. Girish Singhal. Geometrical and Topological Directives for Protein Folding Kinetics - A Relationship Study
6. Mohit Singh. Automated Design of Unnatural Fluorescent Proteins.
7. Amey Muley. Development of Pseudo receptor polygon mesh from Kinase Biophores
8. Arrojwala Manu Tej Sharma. Cheminformatics approaches to elucidate mechanism of action of small molecules.
9. Shubang Shukla. Analysis of Differentially Expressed Proteins in Cancers using Network Theory
10. Anant Sachan. Repurposing of existing drugs for COVID-19.

TEACHING

Courses at IIT Guwahati

Undergraduate Courses (B.Tech Biosciences & Bioengineering)

BT 101 Modern Biology / Introductory Biology

BT 205 Biophysics

BT 301 Bioinformatics and Computational Biology

BT 310 Bioinformatics and Computational Biology Laboratory

BT 305 Computational Biology

BT 301 Biophysics (Revised curriculum)

BT 305 Computational Biology (Revised curriculum)

Graduate Courses (M.Tech and PhD)

BT 601 Analytical Biotechnology

BT 501 Biotechniques

BT 510 Bio-techniques Laboratory

BT 617 Concepts and Methods in Proteomics

BT 610 Frontiers in Biomolecular Simulations

SPONSORED PROJECTS

(Implementing Institute: IIT Guwahati)

No.	Title
1	<p>Mechanistic investigations on the using a efficacy and mode of action of Ashwagandha and Yogaraj Guggulu, hybrid Proteomics-Cheminformatics-Network medicine approach for the treatment of Osteoarthritis</p> <p>Role: PI Present status: Ongoing</p>
2	<p>Design and Characterization of peptide-based cell targeting domains with live cell and animal imaging methods</p> <p>Role: PI Present status: Ongoing</p>
3	<p>Re-purposing of FDA Approved Drugs for TB treatments.</p> <p>Role: Co-PI, PI: Vishal Trivedi Present status: Completed</p>
4	<p>Peptide Based Molecular Constructs for Tumor Homing and Small Molecule Delivery</p> <p>Role: PI Present status: Completed</p>
5	<p>Design, Synthesis and Characterization of Metal Impregnating Nano-assemblies using Peptide Model Systems; Applications in heavy metal entrapment in North-East Region.</p> <p>Role: PI Present status: Completed</p>
6	<p>Mechanistic insights into IAPP self-assembly, targeting early intermediates for therapeutics</p> <p>Role: PI</p>

	Present status: Completed
7	Design and Characterization of Polypeptide constructs as Prototypes for Bio-sensing and Imaging Applications. Role: PI Present status: Completed
8	Design synthesis and Characterization of self-assembled molecular materials from heterotactic polypeptide constructs. Application in drug delivery and nanoscale energy storage devices. Role: PI, Co-PI: Dr. Senthilkumar S. Present status: Completed
9	Computational engineering of protein folding pathways: Implication on stability, misfolding and aggregation Role: PI, Co-PI: NA Present status: Completed
10	Computational design and experimental verification of self-assembled peptides with unnatural amino-acids as building blocks. Role: PI, Co-PI: NA Present status: Completed

Implementing Institute: IBAB Bangalore

11 Modeling Folding Mechanism of Amyloidogenic Proteins in silico.
Role: Co-PI
Present status: Completed

PATENTS

International Patent

1. Title: A device for non-invasive treatment of neurodegenerative diseases.

Inventors: Vibin Ramakrishnan, Gaurav Pandey, Harshal B. Nemade, Jahnu Saikia, Sajitha S, & Nitin Chaudhary.

Patent No. WO/2019/012556. Present Status: Published

Indian Patents

1. Generation and usage of Di-Histidine based stimulus responsive nanostructures

Inventors: Vibin Ramakrishnan, Sajitha S, Nitin Chaudhary & Gaurav Pandey.

Patent No. 243/KOL/2015. Dated 09.03.2015. Present Status: Published

2. Antimicrobial Peptides.

Inventors: Vibin Ramakrishnan, Prakash Kishore Hazam, Nitin Chaudhary, Vishal Trivedi and Gaurav Jerath.

Patent No. 333/KOL/2015. Dated 26.03.2015. Present Status: Published

3. Antimicrobial short peptides.

Inventors: Nitin Chaudhary, Karabi Saikia, Durga Sravani Yalavarthi and Vibin Ramakrishnan

Patent No. 353/KOL/2015. Dated 30.03.2015, Present Status: Published

4. Title: Magnetic hydrocarbon crystals

Inventors: Vibin Ramakrishnan, Sajitha S, Nitin Chaudhary & Gaurav Pandey.

Patent No. 201631011471 Dated 31.03.2016.

5. Title: Peptide based Molecular Constructs for Tumor Homing and Cell Penetration

Inventors: Vibin Ramakrishnan, Ruchika Goyal and Gaurav Jerath

Patent No. TEMP/E-1/36058/2019-KOL Dated 23.08.2019

6. Title: Peptide-based Drug Delivery Vectors

Inventors: Vibin Ramakrishnan and Gaurav Jerath

Patent No. TEMP/E-1/36087/2019-KOL Dated 23.08.2019

7. Title: Peptide based modulators for amyloidogenic diseases

Inventors: Vibin Ramakrishnan, Gaurav Pandey and Vivek Prakash

Patent No. TEMP/E-1/36478/2019-KOL Dated 27.08.2019

8. Title: Amalaki Rasayana constituents for the treatment of cardiac hypertrophy

Inventors: Vibin Ramakrishnan, Aparna Rai

Patent No. TEMP/E1/28937/2020-KOL Dated 22.06.2020

9. Title: Repositioning of Existing Drug Molecules for Treatment of Cardiac Hypertrophy

Inventors: Vibin Ramakrishnan, Aparna Rai

Patent No. TEMP/E1/28939/2020-KOL Dated 22.06.2020

PUBLICATIONS (Books)

1. De Novo Peptide Design: Principles and Applications

Editors: Vibin Ramakrishnan, Kirti Patel & Ruchika Goyal



Publisher: Elsevier, UK

Present status & Publication Date

Complete, Publication Date: September 2022

This book is expected to provide useful insights in understanding the governing principles of peptide design and its applications in various fields of science.

2. Biophysical Characterization of Functional Peptides.

Editor: Vibin Ramakrishnan

**SPRINGER
NATURE**

**Publisher: Springer Nature,
USA**

Present status & Publication Date (Projected):

Springer approved the project, Contract signed, Publication Date: Not finalized

This book details the biophysical characterization of peptide materials for four actively pursued areas in peptide science.

PUBLICATIONS (Refereed Journals)

(* indicates Corresponding author)

1. Vivek Prakash, Yvonne Christian, Amay Sanjay Redkar, Abhishek Roy, R. Anandalakshmi and Vibin Ramakrishnan*. Antibacterial Hydrogels of Aromatic Tripeptides. *Soft Matter* (2022) DOI : 10.1039/D2SM00606E/

Publisher: **Royal Society of Chemistry**

2. Gaurav Jerath, Pramod Darvin, Yvonne Christian, Vishal Trivedi, T. R. Santhosh Kumar and Vibin Ramakrishnan*. Delivery of Small Molecules by Syndiotactic Peptides for Breast Cancer Therapy. *Molecular Pharmaceutics* (2022) DOI: acs.molpharmaceut.2c00238

Publisher: **American Chemical Society**

3. Vivek Prakash, Mukesh B, Sajitha Sasidharan, Amay Sanjay Redkar, Abhishek Roy, R. Anandalakshmi and Vibin Ramakrishnan*. Syndiotactic hexamer peptide nanodots. *European Biophysics Journal* (2022) DOI : 10.1007/s00249-022-01610-3

Publisher: **Springer**

4. Sajitha Sasidharan, Sayandeep Ghosh, Rishi Sreedhar, Kalpana Kumari, Subhash Thota, and Vibin Ramakrishnan*. Anisotropic Ferromagnetic Organic Nanoflowers, *Journal of Physical Chemistry C* (2022) DOI: 10.1021/acs.jpcc.2c01462.

Publisher: **American Chemical Society**

5. Jahnu Saikia, Venugopal T Bhat, Lokeswara Rao Potnuru, Amay S Redkar, Vipin Agarwal, Vibin Ramakrishnan*. Minimalist de novo design of an artificial enzyme. *ACS Omega* (2022), accepted, in press

Publisher: **American Chemical Society**

6. Jahnu Saikia, K. Dharmalingam, R. Anandalakshmi, Amay Sanjay Redkar, Venugopal T. Bhat and Vibin Ramakrishnan*, Electric Field Modulated Peptide based Hydrogel Nanocatalyst, *Soft Matter* (2021) DOI: 10.1039/D1SM00724F

Publisher: **Royal Society of Chemistry**

7. Ruchika Goyal, Gaurav Jerath, Aneesh Chandrasekharan, Yvonne Christian, T. R. Santhoshkumar, and Vibin Ramakrishnan*, Molecular hybridization combining tumor homing and penetrating peptide domains for cellular targeting, **Drug Delivery and Translational Research** (2021) DOI : 10.1007/s13346-021-01035-z
Publisher: **Springer**
8. Ruchika Goyal, Gaurav Jerath, Akhil R., Aneesh Chandrasekharan, Eswara Rao Puppala, Srikanth Ponneganti, Anupam Sarma, V.G.M. Naidu, T. R. Santhoshkumar, and Vibin Ramakrishnan* "Geometry Encoded Functional Programming of Tumor Homing Peptides for Targeted Drug Delivery", **Journal of Controlled Release** (2021) DOI: 10.1016/j.jconrel.2021.03.0101
Publisher: **Elsevier**
9. Aparna Rai, Vikas Kumar, Gaurav Jerath, C. C. Kartha & Vibin Ramakrishnan* "Mapping drug-target interactions and synergy in multi-molecular therapeutics for pressure-overload cardiac hypertrophy", **npj Systems Biology and Applications** (2021) DOI: 10.1038/s41540-021-00171-z
Publisher: **Nature (npj)**
10. Prakash Kishore Hazam, Chimanjita Phukan, R. Akhil, Anjali Singh & Vibin Ramakrishnan* "Antimicrobial effects of syndiotactic polypeptides", **Scientific Reports**. (2021) DOI.10.1038/s41598-021-81394-2
Publisher: **Nature (npj)**
11. Vivek Prakash, Ranjit Ranbhor and Vibin Ramakrishnan* "De novo designed Hetero-chiral Blue Fluorescent Protein", **ACS Omega** (2020) DOI:10.1021/acsomega.0c02574
Publisher: **American Chemical Society**
12. Ruchika Goyal, Gaurav Jerath, Aneesh Chandrasekharan, T. R. Santhosh Kumar and Vibin Ramakrishnan* "Peptide-based delivery vectors with pre-defined geometrical locks", **RSC Medicinal Chemistry** (2020). DOI.10.1039/d0md00229a
Publisher: **Royal Society of Chemistry**
13. Gaurav Pandey & Vibin Ramakrishnan*. Invasive and non-invasive therapies for Alzheimer's disease and other amyloidosis. **Biophysical Reviews** (2020). DOI.10.1007/s12551-020-00752-y
Publisher: **Springer**

14. Gaurav Jerath, Ruchika Goyal, Vishal Trivedi, T R. Santhoshkumar, Vibin Ramakrishnan*. Conformationally constrained peptides for drug delivery. **Journal of Peptide Science**. (2020) DOI: 10.1002/psc.3244
Publisher: **Wiley**

15. Modulation of tau protein aggregation using ‘Trojan’ sequences. Gaurav Pandey, Sudhir Morla, Sachin Kumar, Vibin Ramakrishnan*. **Biochimica et Biophysica Acta, BBA - General Subjects** (2020). DOI: 10.1016/j.bbagen.2020.129569.
Publisher: **Elsevier**

16. Modulating A β Fibrillogenesis with ‘Trojan’ peptides. Gaurav Pandey, Sudhir Morla, Sachin Kumar, Vibin Ramakrishnan*. **Neuropeptides** (2020) DOI: 10.1016/j.npep.2020.102030.
Publisher: **Elsevier**

17. Directive effect of chain length in modulating peptide nano-assemblies. Gaurav Pandey, Prem Prakash Das, Vibin Ramakrishnan*. **Protein & Peptide Letters** (2020) DOI: 10.2174/0929866527666200224114627.
Publisher: **Bentham Science**

18. Praksah Kishore Hazam, Akhil, R., Gaurav Jerath, Jahnu Saikia and Vibin Ramakrishnan. Topological effects on the designability and bactericidal potency of antimicrobial peptides. **Biophysical Chemistry**, 2019, 142, 10 – 18.
Publisher: **Elsevier**

19. Jahnu Saikia, Gaurav Pandey, Sajitha Sasidharan, Ferrin Antony, Harshal B. Nemade, Sachin Kumar, Nitin Chaudhary, and Vibin Ramakrishnan*. Electric Field Disrupts Amyloid Aggregation; Potential Non-invasive Therapy for Alzheimer’s Disease. **ACS Chemical Neuroscience**. (2019), doi:10.1021/acschemneuro.8b00490.
Publisher: **American Chemical Society**

20. Gaurav Pandey, Sudhir Morla, Harshal B. Nemade, Sachin Kumar and Vibin Ramakrishnan*. Modulation of Aggregation with Electric Field; Scientific Roadmap for a Potential Non-Invasive Therapy Against Tauopathies. **RSC Advances**. (2019), doi: 10.1039/c8ra09993f.
Publisher: **Royal Society of Chemistry**

21. Gaurav Jerath, Ruchika Goyal, Vishal Trivedi T.R. Santhoshkumar and Vibin Ramakrishnan*. Syndiotactic Peptides for Targeted Delivery. **Acta Biomaterialia**. (2019), doi: 10.1016/j.actbio.2019.01.036.
Publisher: **Elsevier**
22. Sooram Banesh, Vibin Ramakrishnan, and Vishal Trivedi. Mapping of phosphatidylserine recognition region on CD36 ectodomain. **Archives of Biochemistry and Biophysics**. (2018), doi:10.1016/j.abb.2018.10.005.
Publisher: **Elsevier**
23. Ranbhor Ranjit, Anil Kumar, Abhijit Tendulkar, Kirti Patel, Vibin Ramakrishnan*, and Susheel Durani. IDeAS: Automated Design Tool for Hetero-chiral Protein Folds. **Physical biology**. (2018), doi:10.1088/1478-3975/aacdc3.
Publisher: **Institute of Physics (IOP)**
24. Prakash Kishore Hazam, Anjali Singh, Nitin Chaudhary and Vibin Ramakrishnan*. Bactericidal Potency and Extended Serum Life of Stereo-Chemically Engineered Peptides Against Mycobacterium. **International Journal of Peptide Research and Therapeutics**. (2018), doi:10.1007/s10989-018-9690-0.
Publisher: **Springer**
25. Ranbhor Ranjit, Anil Kumar, Kirti Patel, Vibin Ramakrishnan*, and Susheel Durani. Automated design evolution of stereo-chemically randomized protein foldamers. **Physical biology**. (2018), doi:10.1088/1478-3975/aaac9a
Publisher: **Institute of Physics (IOP)**
26. Sajitha Sasidharan, Shyni P. C., Nitin Chaudhary, and Vibin Ramakrishnan*. Single Crystal Organic Nanoflowers. **Scientific Reports**. (2017), doi:10.1038/s41598-017-17538-0.
Publisher: **Nature (npj)**
27. Prakash Kishore Hazam, Gaurav Jerath, Nitin Chaudhary, and Vibin Ramakrishnan*. Peptidomimetic Approach in the Design of Syndiotactic Antimicrobial Peptides. **International Journal of Peptide Research and Therapeutics**. (2017), doi:10.1007/s10989-017-9615-3
Publisher: **Springer**

28. Prakash Kishore Hazam, Gaurav Jerath, Anil Kumar, Nitin Chaudhary, and Vibin Ramakrishnan*. Effect of tacticity-derived topological constraints in bactericidal peptides. **Biochimica et Biophysica Acta**. (2017), doi:10.1016/j.bbamem.2017.05.002.
Publisher: **Elsevier**

29. Gaurav Pandey, Jahnu Saikia, Sajitha Sasidharan, Deep C. Joshi, Subhash Thota, Harshal B. Nemade, Nitin Chaudhary, and Vibin Ramakrishnan*. Modulation of Peptide Based Nano-Assemblies with Electric and Magnetic Fields. **Scientific Reports**. (2017). doi:10.1038/s41598-017-02609-z
Publisher: **Nature (npj)**

30. Karabi Saikia, Yalavarthi Durga Sravani, Vibin Ramakrishnan, and Nitin Chaudhary.
Highly potent antimicrobial peptides from N-terminal membrane-binding region of E. coli MreB. **Scientific Reports**. (2017), 7, 42994. DOI:10.1038/srep42994.
Publisher: **Nature (npj)**

31. Sajitha Sasidharan, Prakash Kishore Hazam and Vibin Ramakrishnan*. Symmetry Directed Self-Organization in Peptide Nano-Assemblies Through Aromatic pi-pi Interactions. **The Journal of Physical Chemistry B**. (2017) 121, 404–411. DOI: 10.1021/acs.jpcc.6b09474.
Publisher: **American Chemical Society**

32. Anil Kumar, Ranjit Ranbhor, Kirti Patel, Vibin Ramakrishnan*, Susheel Durani. Automated Protein and Peptide Design: Landmarks and Operational Principles. **Progress in Biophysics and Molecular Biology**. (2016). DOI:http://dx.doi.org/10.1016/j.pbiomolbio.2016.12.002.
Publisher: **Elsevier**

33. Suman Jyoti Deka, Ashalata Roy, Vibin Ramakrishnan, Debasis Manna and Vishal Trivedi. Danazol has potential to cause pkc translocation, cell-cycle dysregulation and apoptosis in breast cancer cells. **Chem. Biol. Drug Des.** (2016) DOI:10.1111/cbdd.12921.
Publisher: **Wiley**

34. Gaurav Jerath, Prakash Kishore Hazam, Shashi Shekhar, Vibin Ramakrishnan*. Mapping the Geometric Evolution of Protein Folding Motor. **PLOS ONE**. (2016) 11(10): e0163993. DOI:10.1371/journal.pone.0163993.

Publisher: **PLOS**

35. A. Mehra, Gaurav Jerath, Vibin Ramakrishnan, Vishal Trivedi. Characterization of ICAM-1 biophore to design cytoadherence blocking peptides. **Journal of Molecular Graphics & Modelling**. (2015) 57, 27-35.

Publisher: **Elsevier**

36. Gaurav Jerath, Prakash Kishore Hazam and Vibin Ramakrishnan*. bPE toolkit: toolkit for computational protein engineering. **Systems and Synthetic Biology**. (2014) 8:337-341.

Publisher: **Springer**

37. Rahul Metri, Gaurav Jerath, Govind Kailas, Adityabarna Pal & Vibin Ramakrishnan*. Structure Based Barcoding of Proteins. **Protein Science** (2014) 23, 117-120.

Publisher: **Wiley**

38. Kimjolly Lhouvum.; Vibin Ramakrishnan & Vishal Trivedi. Insight into structural and biochemical determinants of substrate specificity of PFI1625c: Correlation analysis of protein-peptide molecular models. **Journal of Molecular Graphics & Modelling** (2013) 43, 21-30.

Publisher: **Elsevier**

39. Vibin Ramakrishnan, Saeed Salem; Saipraveen Srinivasan, Mohammed Zaki, Suzanne Mathews, Wilfredo Colon and Christopher Bystroff. Developing a detailed mechanistic model for protein unfolding. **Proteins: Structure Function & Bioinformatics** (2012), 80, 920-934.

Publisher: **Wiley**

40. Anil Kumar and Vibin Ramakrishnan*. Alternate protein scripts with unnatural alphabets. **Systems & Synthetic Biology** (2010), 4(4), 247-256.

Publisher: **Springer**

41. Aimy Sebastian, Andreas Bender and Vibin Ramakrishnan*; Virtual Activity Profiling of Bioactive Molecules by 1D Fingerprinting. **Molecular Informatics** 51 (2010) 29, 773-779.

Publisher: **Wiley**

42. Anil Kumar; Vibin Ramakrishnan; Ranjit Ranbhor and Susheel Durani. Homochiral Stereochemistry: The Missing Link of Structure to Energetics in Protein Folding. **Journal of Physical Chemistry B** (2009) 113 (51), pp 16435–16442.

Publisher: **American Chemical Society**

43. Ranjit Ranbhor; Vibin Ramakrishnan; Anil Kumar and Susheel Durani. The Interplay of Sequence and Stereochemistry in defining Conformation in Proteins and Polypeptides. **Biopolymers** (2006) 83, 537-545.

Publisher: **Wiley**

44. Vibin Ramakrishnan; Ranjit Ranbhor; Anil Kumar and Susheel Durani. The link between Sequence and Conformation in Protein Structures appears to be Stereochemically Established. **The Journal of Physical Chemistry B** (2006) 110, 9314-9323.

Publisher: **American Chemical Society**

45. Vibin Ramakrishnan; Ranjit Ranbhor and Susheel Durani. Probing Main Chain Roles in Protein Structure and Folding Stereochemically. A Simulated Annealing Folding Study of Isotactic, Syndiotactic and Heterotactic Polypeptides. **Biopolymers** (2005) 78, 96-105.

Publisher: **Wiley**

46. Vibin Ramakrishnan; Ranjit Ranbhor and Susheel Durani. Existence of Specific "Folds" in Polyproline-II Ensembles of an Unfolded Alanine Peptide Detected by Molecular Dynamics. **Journal of the American Chemical Society** (2004) 126, 16332-16333.

Publisher: **American Chemical Society**

Reviews and Book Chapters

47. Praksah Kishore Hazam, Ruchika Goyal, Vibin Ramakrishnan*. Peptide based Antimicrobials: Design Strategies and Therapeutic Potential. **Progress in Biophysics and Molecular Biology**. (2018) <http://doi.org/10.1016/j.pbiomolbio.2018.08.006>

Publisher: **Elsevier**

48. Gaurav Jerath & Vibin Ramakrishnan*. Web-resources in Post Genomic Era. **Health Sciences** (2014) 1(3), JS002A.

49. Sajitha Sasidharan & Vibin Ramakrishnan. Aromatic interactions directing peptide nano-assembly. **Advances in Protein Chemistry and Structural Biology** (2022) DOI: 10.1016/bs.apcsb.2022.01.001.

Publisher: Academic Press, Elsevier.

50. Ruchika Goyal & Vibin Ramakrishnan. Peptide-Based Drug Delivery Systems. Characterization and Biology of Nanomaterials for Drug Delivery. Elsevier (Book Chapter, 2018). ISBN: 978-0-12-814031-4

Publisher: Elsevier.

51. Aimy Sebastian & Vibin Ramakrishnan*. Computational Biology Applications. **Nutri Horticulture**. Ed. K. V. Peter. DPH New Delhi. (2012) pp 123-142.

Publisher: NIPA.

COMPUTATIONAL TOOLS / WEB SERVERS

1. Protein Barcode

Description: Tool structure based barcoding of proteins (**MID, IIT Guwahati**)

Reference: Structure Based Barcoding of Proteins Rahul Metri, Gaurav Jerath, Govind Kailas, Nitin Gachhe , Adityabarna Pal & Vibin Ramakrishnan (2014) **Protein Science** 23:117–120 (Cover page)



2. Basic Protein Engineering Toolkit (bPE Toolkit, MID IIT Guwahati)

Description: Consists of six useful protein modeling tools

Reference: bPE toolkit: Toolkit for Computational Protein Engineering Gaurav Jerath, Prakash K. Hazam and Vibin Ramakrishnan. **Systems and Synthetic Biology**. (2014) 8:337–341.

3. Geofold: Protein Unfolding Pathway prediction server (Bystroff Lab, RPI New York)

Description: Tool for predicting protein unfolding pathways

Reference: Vibin Ramakrishnan, Saeed Salem; Saipraveen Srinivasan, Mohammed Zaki, Suzanne Mathews, Wilfredo Colon and Christopher Bystroff. **Proteins: Structure Function & Bioinformatics** (2012), 80, 920-934.

4. IDEAS (Durani Lab, IIT Bombay)

Description: Software for protein inverse design

Reference: Ranbhor Ranjit, Anil Kumar, Abhijit Tendulkar, Kirti Patel, Vibin Ramakrishnan*, and Susheel Durani. IDeAS: Automated Design Tool for Hetero-chiral Protein Folds. **Physical biology**. (2018), doi::10.1088/1478-3975/aacdc3

5. Time Piece model for Virtual Activity Profiling of Drug molecules (Vibin Ramakrishnan Lab, IBAB Bangalore)

Description: Tool virtual activity profiling of drugs.

Reference: Aimy Sebastian, Andreas Bender and Vibin Ramakrishnan*; Virtual Activity Profiling of Bioactive Molecules by 1D Fingerprinting. **Molecular Informatics** (2010) 29, 773-779.

CONFERENCE PRESENTATIONS (SELECTED)

1. Vibin Ramakrishnan, Ranjit Ranbhor and Susheel Durani. Stereochemical origins of compactness and stability in proteins. A simulated annealing study of poly L and alternating L, D diastereomer variants of Ac-Ala₃₀-NHMe. *48th Annual Meeting of Biophysical Society, Baltimore, Maryland, USA. Biophys. J S.* 2004, 86, 621.
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11. Ranjit Ranbhor, Vibin Ramakrishnan, Anil Kumar, Abhijit Tendulkar and Susheel Durani. Computational Design of Heterochiral Protein Assemblies. *75th Annual Meeting, Society of Biological Chemists (India) December 8-11, 2006* at Jawaharlal Nehru University, New Delhi.
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INVITED LECTURES (SELECTED)

1. Symmetry directed self-organization of nano-assemblies through aromatic π - π interactions. International Conference on Nanomaterials: Synthesis, Characterization and Applications (ICNP 2018).MGU, December 9, 2018.
2. Design of Novel Hetero-Tactic Fluorescent Proteins by Automated Design Approaches. INPEC 2017: The 23rd INPEC Meeting: Protein Structure, Function and Engineering, November 11, 2017, Bose Institute, Kolkata.
3. A Reductionist Approach to Drug Discovery Research. National Workshop on Drug Design and Discovery, ILS Bhubaneswar, March 22, 2017
4. Ying-yang hypothesis for conformational fold selection and its implications in designing peptide assemblies. Third International conference on Natural Polymers, Biopolymers ICNP 2012. MG Univ.
5. Topology based prediction of Protein folding pathways.Workshop on modeling biological systems II. Indian Statistical Institute, Kolkata & Mizoram University, Aizwal. 2012.
6. Canonicalization of Molecular Structures for Virtual Activity Profiling. National workshop on Chemical Informatics; Applications in Drug Design. Tezpur University. 2012.
7. A 'reductionist' approach in virtual activity profiling of drug molecules **ICDDT**, 2011. 3rd International Conference on Drug Discovery and Therapy, Feb 7-10, 2011 Dubai, UAE.

8. Computational Protein Design. ADCOM 2009. International Conference on advanced computing and communication. Indian Institute of Science Bangalore. 14-17 Dec 2009.

EDITORIAL BOARD MEMBERSHIP

1. Editorial Board Member, **Scientific Reports**. 2018 onwards.

Publisher: **Nature Publishing Group, Springer Nature** (npj journal). Impact Factor: 4.379



2. Editorial Board Member, **Journal of Controlled Release**, 2021 onwards

Publisher: **Elsevier**, Impact Factor: 9.776



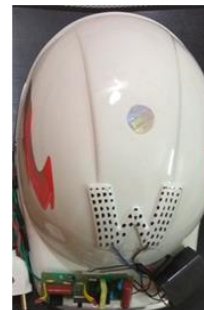
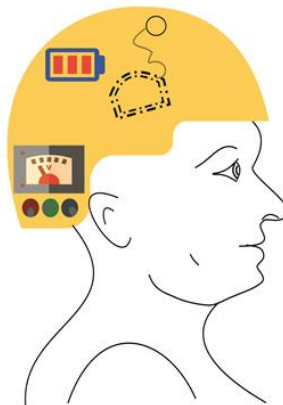
TECHNOLOGIES DEVELOPED AND IT'S SOCIETAL IMPACT

Research stories in Newspapers (Media)

1. Electric field based device for the treatment of Alzheimer's Disease

Alzheimer's disease (AD) is the most prevalent form of dementia in the elder population, affecting 48 million people worldwide. Alzheimer's Association estimates one new case every 33 seconds. This number may almost triple by 2050 in the absence of any cure or prevention methods. Although dementia mainly affects older people, it is not a normal part of ageing. AD currently has no available cure. Most of the neurodegenerative diseases such as Alzheimer's disease are characterized by selective loss or degeneration of specific regions of the brain, triggered by accumulation of protein or peptide aggregates. Approximately hundred potential drugs for treatment of Alzheimer's disease have failed between 1998 and 2011, which shows the gravity of the problem.

Two separate studies conducted by Gaurav Pandey and Jahnu Saikia under the supervision of Prof. Vibin Ramakrishnan and Prof. Harshal Nemade at Indian Institute of Technology Guwahati, have shown that low voltage electric field can retard the formation and accumulation of toxic neurodegenerative molecules responsible for short term memory loss of Alzheimer's patients. Details of the work have been published in ACS Chemical Neuroscience of American Chemical Society and RSC Advances of Royal Society of Chemistry in 2019. The same group has published couple of more articles this year (2020) in BBA and neuropeptides, exploring the possibility of 'trojan peptides' to intervene aggregation. IIT Guwahati has filed an international patent for the discovery.



AD Helmet: Prototype of a futuristic device

Upon exposure to electric field, we could retard the degeneration of nerve cells to an extent of 17 - 35 %. Objectively, this would translate to about 10 years delay in the onset of the disease. Considering the fact that the disease symptoms first appear after the age of 60, and average life expectancy of human population is 72 years, a field based therapy can possibly help to improve the quality of life of an average patient significantly. However, this is just a prototype, and many more trials in animal subjects may be necessary to eventually use it as a therapeutic option.

IIT-Guwahati takes 'Trojan horse' route to fight Alzheimer's disease

Designer peptides to impede aggregation of brain plaque

RAHUL KARMAKAR
GUWAHATI

A war trick borrowed from Greek mythology, specifically poet Homer's epic *Iliad*, could help reduce short-term memory losses associated with Alzheimer's disease.

Researchers at the Indian Institute of Technology-Guwahati (IIT-G) have, after a five-year study, arrived at methods for preventing the accumulation of neurotoxic molecules in the brain, which leads to memory loss.

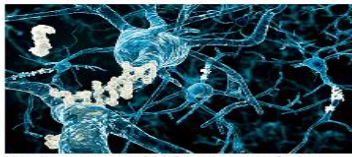
One is the use of "trojan peptides" that does what the Trojan horse did for the ancient Greeks in their victory over Troy.

The other is the application of a low-voltage electric field toward preventing amyloid plaques from aggregating to cause memory loss.

The cause of Alzheimer's is the accumulation of amyloid-beta peptides in the brain.

"This peptide is akin to the plaque that blocks arteries over a period of time, affecting blood supply and leading to cardiovascular diseases. Its aggregation, meaning the formation of one over the other, deforms the cortex of the brain leading to Alzheimer's," Vibin Ramakrishnan of IIT-G's Department of Biosciences and Bioengineering, told *The Hindu*.

He teamed up with Pro-



Slow degeneration: Amyloid plaques on axons of neurons affected by Alzheimer's disease. -serrymoskovskoyev

fessor Harshat Nemade of IIT-G's Department of Electronics and Electrical Engineering, and research scholars Gaurav Pandey and Jahnvi Saikia, for the study on the neurochemical principles of Alzheimer's disease and ways of arresting it.

The peptide molecules need to have a certain structure to aggregate.

The use of an external electric or magnetic field modulates these molecules to "pull back the possibility of Alzheimer's to a certain extent".

The second approach has been to design a "deceitful" peptide with "negative syntactical points" for checking the plaque formation.

"The trojan peptide is roughly like the peptide in the body. But while it goes along with the other peptides, its function is contrary

to aggregation. Through intravenous injection of the trojan peptide, we can retard the degeneration of nerve cells by 17-35%, translating into a 10-year delay in the onset of the disease," Dr. Ramakrishnan said.

Next step

The next step for the researchers is to work with these techniques on mice induced with Alzheimer's at the National Institute of Pharmaceutical Education and Research in Guwahati.

The IIT-G researchers said some 100 potential drugs for the treatment of Alzheimer's disease failed between 1998 and 2011.

The development of a cure for the disease is important for India, which is third behind China and the U.S. in the number of Alzheimer's patients, they said.

IIT-G researchers make headway in delaying onset of Alzheimer's disease

Assam Tribune

GUWAHATI, May 20: Researchers at the Indian Institute of Technology-Guwahati (IIT-G) have, after a five-year study, arrived at methods for preventing the accumulation of neurotoxic molecules in the brain, which leads to memory loss.

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ASSAM TRIBUNE

Home / Education / IIT Guwahati finds new ways to prevent memory loss due to Alzheimer's

EDUCATION

IIT Guwahati finds new ways to prevent memory loss due to Alzheimer's

The research team explored new ways to prevent the accumulation of neurotoxic molecules in the brain that are associated with short-term memory loss due to Alzheimer's disease.

Guwahati | By Indo Asian News Service
PUBLISHED ON MAY 20, 2020 01:35 PM IST



Representational image.(Unsplash)

Indian Institute of Technology Guwahati (IIT-G) on Wednesday said its researchers have discovered new ways that can help prevent or reduce short-term memory losses associated with the Alzheimers disease.

HINDUSTAN TIMES 20 May, 2020

THE HINDU, 20 May 2020

IIT finds way to prevent Alzheimer's

IIT-Guwahati researchers claimed that they have worked on ideas that can help prevent or reduce short-term memory loss associated with Alzheimer's disease. They studied the neurochemical principles of Alzheimer's and explored new ways to prevent accumulation of neurotoxic molecules in the brain that are associated with short-term memory loss. The IIT team reported methods such as application of low-voltage electric field and the use of "Trojan peptides" to arrest the aggregation of neurotoxic molecules in the brain.

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New Indian Express

The Morning Standard

THIS STORY IS FROM MAY 21, 2020

IIT Guwahati researchers discover new ways to prevent memory loss due to Alzheimer's disease

TIMESOFINDIA.COM | May 21, 2020, 20:54 IST



NEW DELHI: Researchers at Indian Institute of Technology (IIT) Guwahati have found a new way to reduce short-term memory losses associated with Alzheimer's disease. The research team headed by professor Vibin Ramakrishnan and professor Harshat Nemade, of IIT Guwahati studied the neurochemical principles of Alzheimer's, and explored new

ways to prevent accumulation of neurotoxic molecules in the brain that are associated with short-term memory loss.

One of the key reasons for memory loss in Alzheimer's disease is the accumulation of "amyloid beta peptides" in the brain. The professors were looking at methods to reduce the accumulation of these peptides, in order to check the disease.

Times of India 21 May 2020

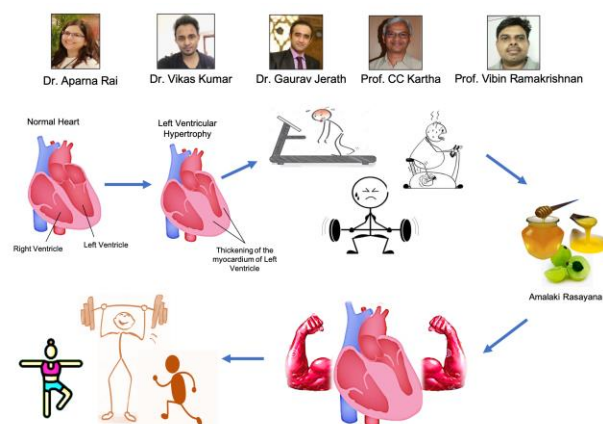
2. Investigation on the therapeutic action of Ayurvedic formulations through modern drug development tools

Professor Vibin Ramakrishnan of IIT Guwahati and Professor C.C. Kartha of Academy of Cardiovascular Sciences have used the principles of Network Pharmacology and Chemoinformatics to analyse the possible targets of components of an Ayurvedic rasayana. In their study recently published in a Nature partnership journal *Systems Biology and Applications*, they examined the efficacy of *Amalaki Rasayana*, an ayurvedic rejuvenating medicine in reducing high blood pressure induced structural and functional changes in the heart. In an earlier study, long term oral intake of *Amalaki rasayana* was found to lessen heart muscle thickening and improve heart function. The present report explains how the rasayana is likely to work in the human body. They employed *in-vivo* studies in small animals, gene-expression and proteomics analysis, informatics tools as well as the techniques of Systems Medicine, which are all followed by those engaged in the discovery of allopathic drugs. They also examined the possible synergy among the actions of different components of the rasayana.

Ayurveda, which means the ‘science of life’, is acknowledged to be practiced in India for at least 5000 years and over one fourth of Indians have been accessing its knowledge for solutions to their health problems. Yet, often we hear that ‘Ayurveda’ is not “scientific”. For the practitioners of modern medicine, ‘scientific evidence’ is synonymous with the results of verification of the efficacy and safety of a potential drug, using the tools and procedures employed in modern medical biology. In the recent conscious efforts to integrate Ayurveda with the principles and practices of modern medicine, what is missing is an approach to contemporize a ‘holistic approach’ as of Ayurveda to the ‘magic bullet’ concept of modern medicine.

For new drug discovery, Modern Medicine has followed, the concept of ‘one gene, one target and one drug’. This approach necessitates identification of single targets in mechanisms that cause diseases. While this is evident in infectious diseases, in cancer, diabetes, cardiovascular diseases and

several other chronic diseases, disease mechanisms involve several molecules and functional pathways. Recent advancements in Systems Biology and Network Medicine have led to the development of the discipline of Network Pharmacology, leading to a paradigm shift in the process of drug discovery. Network Pharmacology is considered more effective for developing multi-component therapeutics. Its tools are also advantageous for the analysis of drug combinations. Traditional Chinese Medicines have been analysed using this novel approach. Similar to other traditional medicines, Ayurvedic medicines are also mostly multi-component formulations and hence are likely to act on multiple targets and pathways. Evidence for this view is however lacking.



Mechanistic investigation of therapeutic effects of AR in the treatment of Cardiac Hypertrophy

Vibin, Kartha and their colleagues provide evidence for the biological action of the multiple components of *Amalaki rasayana* and indicate their possible targets. Their pioneering approach related to Ayurvedic medicines opens up new avenues for systematically examining the modes of action of Ayurvedic medicines utilizing the scientific protocols of modern pharmacology.

Dr. Ramesh Pokhriyal Nishank @DrRPNishank · Mar 20

.@IITGuwahati's Prof. Vibin Ramakrishnan & Prof. C.C. Kartha have used modern drug development methods to analyse the mode of action of an Ayurvedic rejuvenating medicine - Amalaki Rasayana.

Ministry of Education
Government of India



IIT Guwahati
researchers have developed modern drug development methods to understand therapeutic action of Ayurvedic formulations

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.@IITGuwahati's Prof. Vibin Ramakrishnan & Prof. C.C. Kartha have used modern drug development methods to analyse the mode of action of an Ayurvedic rejuvenating medicine - Amalaki Rasayana.

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Dr. Ramesh Pokhriyal Nishank @DrRPNishank · Mar 20

In their study, they have shown how Amalaki Rasayana reduces high blood pressure-induced structural and functional changes in the heart. Good work by #IITGuwahati professors!



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economytimes.indiatimes.com

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economytimes.indiatimes.com

8 19 80

IIT-Guwahati researchers use modern drug development methods to understand therapeutic action of ayurvedic formulations

By Bikash Singh, ET Bureau • Last Updated: Mar 09, 2021, 11:56 PM IST

Synopsis

Prof. Ramakrishnan and Prof. Kartha had earlier found that long term oral intake of Amalaki Rasayana reduces the thickening of heart muscle and improves heart function. The present study that used the emerging scientific approaches of Network Pharmacology and Chemoinformatics shows how the formulation is likely to work in the human body.

Comment



Prof. Vibin Ramakrishnan, Professor, Department of Biosciences and Bioengineering, IIT Guwahati and Prof. C.C. Kartha of Academy of Cardiovascular Sciences have used modern drug development methods to analyse the mode of action of an Ayurvedic rejuvenating medicine.

The Assam Tribune

Working of ayurvedic medicine analysed through modern methods



In a study Prof Vibin Ramakrishnan and Prof CC Kartha have shown how Amalaki Rasayana reduces high blood pressure-induced structural and functional changes in the heart.

TEAM MEMBERS

GUWAHATI, March 9: Prof Vibin Ramakrishnan, Professor of Biosciences and Bioengineering, IIT Guwahati and Prof C.C. Kartha of the Academy of Cardiovascular Sciences, Thiruvananthapuram, have used modern drug development methods to analyse the mode of action of an Ayurvedic rejuvenating medicine.

In their study, the results of which have been recently published in a partnership journal Systems Biology and Applications, they have shown how Amalaki Rasayana reduces high blood pressure-induced structural and functional changes in the heart.

Network pharmacology analyses the influence of drugs on diseases as a whole rather than the one-gene-one-target-one-drug approach that has been conventionally followed in drug discovery.

Network pharmacology is effective for developing multi-component therapeutics, which is typical of traditional systems like ayurvedic and Chinese medicines. The drugs prescribed to these systems are an multiple targets and pathways.

Chemoinformatics helps in comparing drug molecules using standardised computational tools.

While ayurvedic medicines and their ingredients have been handed down over generations and despite their efficacy, they have not yet been understood in a gene-centric manner in the modern methods of drug development, and the scientists.

"The hallmark of ayurvedic system is the long-standing standardised use that is a holistic approach. It is used for both acute and chronic diseases as an ayurvedic medicine is believed to act synergistically.

By analysing a disease condition, the scientists using network pharmacology and chemoinformatics suggest that Amalaki Rasayana is likely to work in the human body.

The team analysed the mode of action of Amalaki Rasayana, an ayurvedic rejuvenating medicine, which is a combination of various herbs, all of which are known to have a beneficial effect on the heart.

The team concluded that Amalaki Rasayana is likely to work in the human body by acting on multiple targets and pathways.

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> IIT-G develops modern technique to explore actions of Ayurvedic rejuvenating medicine

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IIT-G develops modern technique to explore actions of Ayurvedic rejuvenating medicine

09 March 2021 | News

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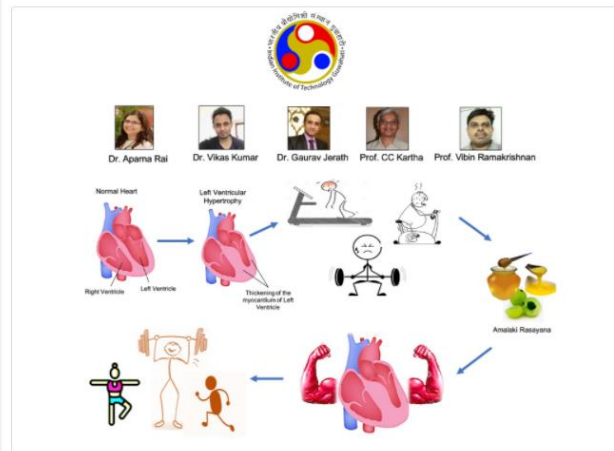
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Prof Ramakrishnan and Prof Kartha had earlier found that long term oral intake of Amalaki Rasayana reduces the thickening of heart muscle and improves heart function



Prof Vibin Ramakrishnan, Professor, Department of Biosciences and Bioengineering, IIT Guwahati (IIT-G) and Prof CC Kartha of Academy of Cardiovascular Sciences (<http://cardiovascularsciences.org/>) have used modern drug development methods to analyse the mode of action of an Ayurvedic rejuvenating medicine - Amalaki Rasayana.

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IIT Guwahati researchers use modern drug development methods to understand therapeutic action of ayurvedic formulations

Our Bureau, Mumbai

Tuesday, March 9, 2021, 14:10 Hrs [IST]

Professor Vibin Ramakrishnan, Professor, Department of Biosciences and Bioengineering, IIT Guwahati and Professor C. C. Kartha of Academy of Cardiovascular Sciences have used modern drug development methods to analyse the mode of action of an ayurvedic rejuvenating medicine - Amalaki Rasayana.

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Network pharmacology analyses the influence of drugs on diseases as a whole rather than the one-gene-one-target-one-drug approach that has been conventionally followed in drug discovery. Network Pharmacology is effective for developing multi-component therapeutics, which is typical of traditional systems like ayurvedic and Chinese medicines – the drugs prescribed in these systems act on multiple targets and pathways. Chemoinformatics helps in comparing drug molecules using standardised computational tools.

While ayurvedic medicines and therapeutics have been handed down over generations and shown anecdotally to be efficacious, they have not yet been subjected to a great extent to the modern methods of drug development. For practitioners of modern medicine, 'scientific evidence' means verification of the efficacy and safety of a potential drug, using the tools and procedures employed in modern medical biology. Thus, Ayurveda is often considered as being 'not scientific'.

"The hallmark of ayurvedic system is the long-standing unverified claim that it is a holistic approach; it treats the body as a whole. Multiple components in an ayurvedic medicine are believed to act synergistically to improve a diseased condition. Our analysis using the tools and techniques of modern medicine suggests that this is, indeed, true," says Prof Ramakrishnan, Professor, Department of Biosciences and Bioengineering, IIT Guwahati.

The scientists employed in-vivo studies in small animals, gene-expression and proteomics analysis, informatics tools and the techniques of Systems Medicine, all of which are used in the development of allopathic drugs. They also examined the possible synergy among the actions of different components of the Rasayana using the Network Pharmacology approach.