



Dr. G. Narahari Sastry

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My goal is to work towards converting knowledge in the areas of computational modelling and artificial intelligence from basic to translational research, by working closely with the society and industry. Ultimately, revitalizing the strength of science and technology is essential in achieving the self-reliant and strong India. In the era of Industry 4.0 and 5.0, combining our traditional wisdom with modern science appear to be indispensable in the sectors such as Education, Health, Agriculture, Industrial and Societal development at large.

Academic Journey and Areas of Research

University of Hyderabad Ph.D. 1994	Israel PDF 1994 - 1996	Switzerland PDF 1996 - 1997	Pondicherry University, Pondicherry 1997 - 2002	CSIR - IICT Hyderabad 2002 - 2019	CSIR - NEIST Jorhat Mar 2019 - Till date
<ul style="list-style-type: none">Quantum chemistryElectronic structure calculations	<ul style="list-style-type: none">Valence Bond ModelingElectron Transfer Reactions	<ul style="list-style-type: none">Theoretical and Physical Organic ChemistryMolecular modeling	<ul style="list-style-type: none">Theoretical and Physical Organic ChemistryMolecular modeling	<ul style="list-style-type: none">Non-covalent InteractionsMaterials modelingBioinformaticsComputer Aided Drug DesignSoftware Development	<ul style="list-style-type: none">Artificial Intelligence and Machine learningSoftware DevelopmentModeling and AI applications in diverse areas (such as Petroleum, genomics, biodiversity, ...)

Awards and Recognitions

- | | |
|---|---|
| <ul style="list-style-type: none">Shanti Swarup Bhatnagar Prize 2011(considered as the highest national recognition in Science)JC Bose National Fellowship, 2015National Bioscience Award of DBT, 2009Swarnajayanthi Fellow of DST, 2005CRSI Medal for excellence in basic research, 2009B. C. Deb Memorial Award for Soil/ Physical Chemistry, Indian Science Congress, 2008B. M. Birla Science prize in Chemistry, 2001Alexander Von Humboldt Fellow, 2006Recognized as the top scientist in several surveys conducted. | <ul style="list-style-type: none">Fellow of Indian National Science Academy (FNA)Fellow of National Academy of Sciences India (FNASc)Fellow of Indian Academy of Sciences (FASc)Fellow of Royal Society of Chemistry (FRSC)Fellow of Biotech Research Society, India (FBRSI)Fellow of Telangana Academy of Sciences (Founder Fellow)Fellow of Andhra Pradesh Akademi of Sciences (FAPAS)Fellow of Association of Biotechnology and Pharmacy (FABP)Life member of: a) World Association of Theoretically Oriented Chemists (WATOC); b) American Chemical Society (ACS); c) Asia-Pacific Conference of Theoretical and Computational Chemistry (APCTCC).International Advisory Board, International Conferences on Noncovalent Interactions (ICNI) |
|---|---|

The above recognitions reveal that G. Narahari Sastry (GNS) is one of the most well recognized scientists of the country working in the interdisciplinary areas of chemistry, biology, material science, and artificial intelligence. In the last decade, GNS group was involved in developing an indigenous software which aims to strengthen the computational drug discovery, and thereby working towards Aatma Nirbhar Bharat. Dr. Sastry is also involved in a number of outreach programs and widely travelled across the globe and has visited over 25 countries.

Google scholar: <https://scholar.google.co.in/citations?user=WsYxRyAAAAJ&hl=en>
ORCID: <https://orcid.org/0000-0003-3181-7673>
Twitter: <https://twitter.com/GNarahariSastry>
Facebook: <https://www.facebook.com/gnarahari.sastry.7>
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Websites: <http://cmm.osdd.net/gnsmmg>, <http://www.neist.res.in/gnsastry>
Wiki: https://en.wikipedia.org/wiki/Garikapati_Narahari_Sastry

Instagram: <https://www.instagram.com/gnsastry>
SRTP website: www.neist.res.in/srtp2020/archivelectures.php
Jigyasa: <http://csirjigyasa.niscair.res.in/>
DDH: <https://innovateindia.mygov.in/ddh2020/>
Inbix/Bioclues: <https://easychair.org/cfp/InBix2021>
Stiner: www.neist.res.in/stiner/aboutSTINER.php
Floriculture: www.neist.res.in/floriculture/

Current Research Activities and Earlier Contributions

Developing indigenous software for drug design, discovery and development with a novel approach, namely disease specific portal development, is one of the most active roles taken by GNS group. This mission is aimed to end overdependency of CADD software, and leads to saving academic institutions spending crores of rupees on buying commercial software. Worked on industrially relevant projects as well as collaborated with Industry.

- With about 300 publications and excellent citations across various disciplines illustrate that the highly interdisciplinary approaches are the integral part of the research group. These research topics strongly connect the four paradigms of science: experimental, theoretical, modelling and data science research.
- Fundamental contributions in supramolecular chemistry which itself is a highly interdisciplinary area.
- Prolific contributions in the area of a) Noncovalent interactions, especially with fundamental contributions in the area of ion-molecule interactions, b) Cooperativity of noncovalent interactions a concept that has been developed by his group, c) Computer aided drug design, d) Aromaticity, e) bucky bowl chemistry f) pericyclic reactions g) Machine learning applications for drug screening, h) Development strategies to model selectivity, permeability and drug molecule screening using dynamic pharmacophore modelling, polypharmacology and network pharmacology approaches.
- Several of the computational predictions from his group are verified experimentally and new experiments are carried out based on the computational methods.
- Trained 27 Ph.D.'s, 20 Postdocs, and over 200 students who carried out projects for various dissertation works such as, M.Tech., M. Pharm, M.Sc., B.Tech. and B. Pharm courses.

Academic Overseas Visits (more than two weeks)

1.	21 May 2018	08 June 2018	Ibaraki University, Japan	Mentor from India for Sakura Science exchange program-2018
2.	08 Jan 2018	13 Jan 2018	Academia Sinica, Taipei, Taiwan	Visiting Professor
3.	19 Aug 2017	05 Sep 2017	Ludwig Maximilians University, Germany	Visiting Professor
4.	18 June 2017	27 June 2017	Institute of Biomedical Chemistry, Moscow and St. Petersburg	Visiting Professor (Indo-Russia DST-RSF project)
5.	28 Apr 2014	01 July 2014	Kyushu University, Japan	Visiting Professor
6.	28 Nov 2011	02 Apr 2012	Institute of Molecular Sciences, Okazaki, Japan	Visiting Professor
7.	22 May 2010	28 May 2010	Institute of Molecular Science, Japan; Gifu University, Japan; Chemical Society of Japan	INSA-JSPS Visiting Scientist & Invited Speaker
8.	11 May 2009	20 May 2009	Institute of Molecular Science, Japan	INSA-JSPS Visiting Scientist
9.	13 Oct 2008	28 Nov 2008	Jackson State University, United States of America	Visiting Scientist
10.	05 June 2008	26 June 2008	Ludwig Maximilians University, Germany	DST-DADD Visiting Scientist
11.	25 Jan 2008	30 Jan 2008	Institute of Molecular Science, Okazaki, Japan	IMS Visiting Researcher
12.	01 July 2006	05 June 2007	Ludwig Maximilians University, Germany	Alexander Von Humboldt Fellow & invited speaker in Germany (Munich, Harburg, Mulheim, Giessen, Berlin, Heidelberg), Netherland (Amsterdam, Leiden), Switzerland (Geneva, Fribourg) and Belgium (Brussels)
13.	01 May 1998	30 July 1998	University of Fribourg, Switzerland	Visiting Scientist

Professional Affiliations and achievements

Delivered more than 450 lectures at different Universities/Institutions and 100 overseas talks in international conferences

- Chairman, Drug Discovery Hackathon Training Committee
- Chairman, Jigyasa Task Force of CSIR
- Chairman, NEEPCO R & D advisory board
- President and Life member of BIOinformatics CLUB for Experimenting Scientists (BIOCLUES)
- Dr. Sastry has peer reviewed several hundreds of publications, involved in the selection of faculty and scientists of a number of premier institutes of the country, he is also assisted in the selection of the most prestigious fellowship and awards of the country.
- Life member of Chemical Research Society of India (CRSI)
- Life member of Andhra Pradesh Akademi of Sciences
- Life member of Indian Biophysical Society
- Highlighting author of highest-quality research in ACS Journals in 2012.
- Life member of Bioinformatics and Drug Discovery Society (BIDDS)
- Adjunct Faculty, NIPER, Kolkata
- Member (EX-officio) of Board of Governors, NIPER, Guwahati
- Member of Working Group of CSIR-Min. of AYUSH
- Member of High-performance computing (HPC) policy committee, CSIR
- Chairman of R&D advisor committee of North Eastern Electrical Power corporation (NEEPCO)
- Member, Scientific & Advisory Committee of Tea Research Association, Tocklai Tea Research Institute, Jorhat
- Member, INSACOG
- Member, Research Council, CSIR-Central Drug Research Institute, Lucknow
- Member, Research Council, CSIR Institute for Himalayan Bioresource Technology, Palampur
- Member, Board of Governors, NIPER Guwahati
- Senate Member, Central Institute of Technology, Kokrajhar
- Member of IQBS, Ibraki University, Japan
- Member, Academic Council, University of Hyderabad
- External Member, IIT Guwahati Senate
- Expert Member, BIRAC- BIG North East Special Call Technical Expert Panel
- Board of studies for Bioinformatics JNTU, Hyderabad
- President of BIOinformatics CLUB for Experimenting Scientists (BIOCLUES)
- Board of studies for Andhra University, Department of Science and Humanities, Vizag
- Board of study member for Vignan Deemed University, Guntur
- On the expert committee of IGNOU-Kerala University sponsored Bioinformatics programs
- Member of research advisory council, Osmania University, Hyderabad
- Board of Studies of Chemistry and Biology of Academy of Scientific & Innovative Research (AcSIR)
- Member of Senate, Academy of Scientific & Innovative Research (AcSIR)
- Expert member, Inorganic and Physical Chemistry Program Advisory Committee to award projects and EMR grants of CSIR
- Member of DST-Women Scientists Scheme-A (WOS-A)
- Indian Institute of Chemical Technology (IICT) Roll of Honour
- IICT Gaurav Sanman
- Best Performance Award for publishing with highest Individual Impact factor in IICT
- Edited special issue on Highlights in Theoretical Chemistry 1 for Theo. Chem. Acc., 2012, 131, 1-215.
- Edited special issue on Computer Aided Drug Design for Ind. J. Chem. A, 2006, 45A, 1-214.
- Reviewer for the following journals: Nature Communications; Nature Chemistry, Chem Rev., J Am. Chem. Soc., J Org. Chem., J Phys. Chem. A & J Phys. Chem. B, Molecular Physics, Current Science (India), Ind. J. Chem. A., Proc. Ind. Acad. Sci. (Chemical Sciences), J. Comp. Chem., Biorg. Med. Chem. Lett., Org. Lett., Chem. Phys. Lett., J. Chem. Sci., Curr. Sci., Chemistry, Tetrahedron, J. Mol. Model., J. Chem. Inf. Mod., J Mol. Graph. Model., Phys. Chem. Chem. Phys., J Biol. Chem., etc
- Member of the editorial advisory board of Journal of Molecular Graphics and Modelling
- Edited special issue on Science for Society for Proceedings of Andhra Pradesh Akademi of Sciences, 2015, 16, 1-162.

Some events organized (selected)

- CSIR Summer Research Training Programme 2020, 16 June – 22 Aug 2020
- Drug Discovery Hackathon 2020 Mentorship and Training programme, 30 September 2021 - 31 March 2022, CSIR-NEIST, Jorhat
- Indian Conference on Bioinformatics (InBIX 2021), 11 - 13 November 2021, CSIR-NEIST, Jorhat
- Drug Discovery Hackathon 2020 Training programme, 13 July 2020 - 12 Sept 2020, CSIR-NEIST, Jorhat
- International Conference on Engineering Sciences & Technologies for Environmental Care (ESTEC-2020), 20-22 Feb 2020, CSIR-NEIST, Jorhat
- Science Communication workshop in association with Welcome Trust/DBT IndiaAlliance, 03 Feb 2020, CSIR-NEIST, Jorhat
- 'Gyantarang' (AcSIR Students' Conference), 23-25 Jan 2020, CSIR-NEIST, Jorhat

- Sensitisation Programme on opportunities for start-ups and entrepreneurs in Agriculture and allied sectors, 27 Jan 2020, CSIR-NEIST in association with NEATEHUB, Jorhat
- Workshop for Chemistry Teachers covering the theme “Periodic Table” under CSIR-KV’s JIGYASA program, Oct 2019
- Nuts and Bolts of Innovation & Entrepreneurship Training Series on "Building & Translating Innovative Ideas", 19-20 Sep 2019, CSIR-NEIST in association with BIRAC-KIIT TBI, Bhubaneswar
- Roadshow on “Brewing Bio-entrepreneurship in Jorhat”, 29 July 2019, CSIR-NEIST in association with BIRAC eastern region team, KIIT Technology Business Incubator, Bhubaneswar
- Interactive session with Defense Research Laboratory (DRL), Tezpur, 2 July 2019
- Interactive workshop between CSIR-NEIST and Gauhati University, 3-4 July 2019, CSIR-NEIST
- International workshop on “Modeling noncovalent interactions in supra/bio catalysis”, 26-30 Aug 2019, Sorbonne University, France and CSIR sponsored by CECAM at Sorbonne University, Paris France
- “Recent Advances in Bioinformatics” national conference at CSIR-NEIST, Jorhat, 23-26 May 2019
- “Innovators cum Entrepreneurs Meet” at CSIR-NEIST, Jorhat, 8-11 May 2019
- “OpenTox 2019 Asia” Conference & Workshop at CSIR-IICT, Hyderabad, 1-3 Mar 2019 [Joint coordinator]
- International conference-cum-workshop on “Informatics Tools in Drug Discovery and Drug Delivery (iTDDD-2018)”, 1-4 Nov 2018 [National Chair]
- One-day workshop on “Machine Learning and Big Data Applications on Drug Repurposing and Chemical Space” at Institute of Chemistry, National Taiwan University, Taiwan on 12 Jan 2018
- “Eighth edition of Asia-Pacific Conference of Theoretical and Computational Chemistry (APCTCC8)”, Indian Institute of Technology Bombay, Mumbai from 15-17Dec 2017 [Chair]
- 9th International Symposium on Computational Methods in Toxicology and Pharmacology integrating Internet resources, 27-30 Oct 2017 [Advisory board member]
- “Modeling chemical and Biological (Re) activity (MCBR-5)” conference, 18-21Feb 2017, CSIR-Central Leather Research Institute in Chennai [Indian Joint Coordinator]
- “The 15th Theoretical Chemistry Symposium (TCS)”, 14-17 Dec 2016, University of Hyderabad, Hyderabad [Convener]
- International conference on Computational Modeling of Molecules and Materials (CM3), 20-22 Oct 2016, Nainital, Uttarakhand, India. [Joint Coordinator]
- Meeting on ‘Development of Informatics for Societal Health Advancement (DISHA): A CSIR lead initiative to bring together doctors, scientists and policy makers on 8 Oct 2016, CSIR-Indian Institute of Chemical Technology, Hyderabad
- Indo-German seminar on “Modeling Chemical and Biological (Re)activity-2015” in Nov 2015, New Delhi [Joint Coordinator]
- Med-Science-2015, an interactive meet of scientists and medical professionals on 8 July 2015, CSIR-Indian Institute of Chemical Technology, Hyderabad

Publications Metrics at a Glance

- **Total no. of publications** ~300
- **Citations** 11,147
- **h-index** 52
- **i10-index** 223
- **Average IF** ~ 4.0

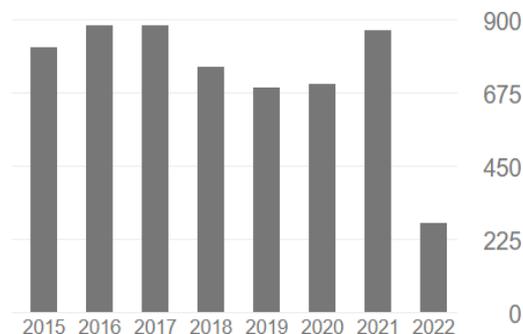
* Some high impact publications

J. Am. Chem. Soc.- 09 (IF 15.4)
 Angew. Chem. Int. Ed.- 04 (IF 15.3)
 Chem. Rev.- 02 (IF 60.6)
 Acc. Chem. Res.- 01 (IF 22.4)

**Publisher-wise Statistics

ACS	64 nos	Elsevier	60 nos
RSC	35 nos	Taylor and Francis	12 nos
WILEY	40 nos	Springer	20 nos

Last eight years' statistics



Source: Google scholar

Major Leadership Activities after taking over CSIR-NEIST

After taking over the leadership at CSIR-NEIST, Jorhat, major activity towards development of campus, capacity and capability building in launching major scientific programs at fundamental and translational level. This involved creation of the state-of-the-art analytical instrumentation, computation and development of experimental facilities for farming and agriculture, animal house, a very exhaustive BSL2 facilities, besides: a) Rural Women Technology Park at CSIR-NEIST supported by DST, Govt. of India; b) CSIR-Centre for Post-Harvest Processing and Research at Itanagar; c) CSIR-NEIST Research Scholars Hostel; d) STINER buildings and Orchidarium; e) Development of first Bamboo Germplasm; f) Recreation of NEEP as “Ecology and Biodiversity Park”; g) Reviving and bring life to about 6 old pilot plants; h) Created two new artificial lakes, and planted over 60,000 trees which is aimed to enhance the rich biodiversity.

- Under the mentorship, Assam has got its first SSB prize: Dr. Binoy K. Saikia, got the highest Indian science Prize in the year 2021, and this is the first time a scientist working in Assam got this recognition. Further several people have got awards, recognitions as well as editorial board memberships, the notable achievements include the fellowships to the scientists in NASI (FNASc), Royal Society of Chemistry (FRSC), CRSI medals, and many more.
- CSIR NEIST received State Science Award 2019 for Science Popularisation and Research. This is received from the honourable CM of Assam and is considered as one of the great recognitions for the institute in the area of science popularization and public outreach.
- A number of initiatives were made to reach farmers, entrepreneurs, students, teachers, researchers and brain storming was done to see how to work towards the development of connectivity between the science and society. CSIR-NEIST secured 1st position in 8th Bhopal Vigyan Mela 2019, jointly organised by Vigyan Bharti, Madhya Pradesh and CSIR-Advanced Material and Processes Research Institute at Bhopal during 13th -16th September 2019.
- While Dr. Sastry is well known for organizing and participating in major national and international events, his leadership after taking over as the director of CSIR-NEIST has provided opportunities to indulge in a number of societal, translational and capacity building initiatives.
- COVID testing facilities were created from the scratch. State of the art genomic facilities are created to tackle the pandemic and INSACOG has recognised CSIR-NEIST as the premier facility center in North-East, 2020.
- One of the most notable events is the conduct of SRTP program which has trained over 15000 students, and 900 lectures were given by eminent mentors all over the country. The top leadership of the country has participated in giving popular science lectures during the pandemic, which has created an atmosphere to greatly inculcate the scientific temper. Besides a number of online and offline seminars were conducted and some series of lectures are given here: a) NEIST Science Forum Lecture; b) Organized set Lectures under ACDS Lecture Series; c) CSIR-NEIST initiated COVID-19 Lecture Series; d) CSIR-NEIST Skill Development Program; e) CSIR- NEIST Diamond Jubilee Lecture Series
- Center for Petroleum Research, Department of Fertilizers, Ministry of Chemical and Fertilizers, 2021
- Established the Regional cum Facilitation Center (RCFC), NMPB at CSIR-NEIST, 2021
- NABL Accreditation for Testing/Analysis services, 2021
- Center of excellence in Advanced Computation and Data Sciences by DBT Govt. of India, 2021
- Established BioNEST Bioincubator at CSIR-NEIST, 2020
- Established the Advanced Computation and Data Sciences division with a team of Scientists from the institute, 2019
- Established Kids world of science, 2019
- STINER (Science and Technology Intervention for North East Region), a DoNER sponsored project with a hub and spoke model is being led, with the hub at NEIST, Jorhat along with the spokes in each of the 8 states of North East.
- 15 multilocational experimental trail for medicinal, aromatic and fruit plants were established to examine the feasibility, viability and cost benefit to farmers. This is led as a part of the Aroma, Floriculture, RCFC and Immunity mission of the institute (2019-2021)

Personal Details

Date of Birth	: 17th January 1966
Permanent Address	: 14/137/1/1A, Raja Srinivas Nagar, Malkajigiri, Hyderabad 500 047, India
Marital Status	: Married, Dr. G. Madhavi Sastry, Senior Director, Schrodinger Mr. G. Nischay Kaushik, Ph.D. in Material Science from IIT Madras Mr. G. Sasank, Ph.D. in Electrical Engineering, Columbia University, N

ABirds-eye View of Selected Fundamental and Academic Contributions

Molecular Property Diagnostic Suite (MPDS) Strengthening Computational Drug Discovery in India <http://mpds.neist.res.in/>

Architecture

- Galaxy interface
- Web browser
- Scripts in Perl, Python, C++ etc.
- MySQL Database
- Chemical Space
- Biological Space
- Chemical Space
- Biological Space
- Disease-Specific Data
- Molecular Modeling, Chemoinformatics, Bioinformatics tools

Data Processing

- Data library: Pubchem, ChEMBL, DrugBank, etc.
- MPDS Target Library
- Identification of new drug targets
- File based contacts
- Deconvolution
- Chemical Analysis
- Drug Activity (MolTox)
- Toxicity (MolTox)
- Biological Activity (MolTox)
- Molecular Docking (MolDock)
- Visualization (MolView)

Data Analysis

- Drug Activity (MolTox)
- Toxicity (MolTox)
- Biological Activity (MolTox)
- Molecular Docking (MolDock)
- Visualization (MolView)

Open source drug discovery tools in MPDS Platform

Housed @ CSIR - NEIST

Advanced Data Driven Modules

- Publicly available databases: Bioassay, ChEMBL, ZINC15, Pubchem, etc.
- Data cleaning and processing
- Encoding structures to mathematical and graph based properties
- Feature selection and extraction
- Classification Models: Random forest, Gradient Boosting, Ensemble classifiers
- Clustering analysis: DBSCAN, SC3M, K-means, Hierarchical
- Text mining and Natural language Processing of MeSH like keywords
- Antimal model
- Membrane permeability
- Toxicity Prediction
- Protein-Ligand interaction analysis

Noncovalent Interactions and Cooperativity

Cooperativity of different Noncovalent Interactions

- Hydrogen Bond
- Halogen bonds
- London pair- π
- Cooperativity
- Single catalyst
- Two catalysts
- Included exclusively by Noncovalent interactions
- Unselective Product Formation
- Selective Product Formation
- Enantioselective transformation using profit solvents and electron-deficient diaryl ureas
- Catalysis
- Biology
- Supramolecular Aggregation

Graphene

- CNT (5,5)
- CNT (4,4)
- CNT (3,3)
- curvature
- BE
- Stronger cation- π as well as hydrogen bonding!

Computer Aided Drug Design

CADD @ GNS GROUP

- Docking
- Virtual Screening
- Molecular Dynamics Simulation
- Molecular Mechanics (MM)
- QSAR
- Drug

Publications:

- Phys. Chem. Chem. Phys., 2012
- Phys. Chem. Chem. Phys., 2011
- Mixed QM/MM
- Met. Inform., 2016
- PLoS ONE, 2014
- Med. Chem. Res., 2014
- J. Mol. Model., 2012
- Met. Inf., 2012
- J. Chem. Inf. Model., 2011
- J. Chem. Inf. Model., 2011
- Med. Chem. Commun., 2011
- Comput. Biol. Chem., 2006
- Ind. J. Chem. A., 2006
- J. Chem. Sci., 2016
- J. Mol. Graph. Model., 2012
- Comb. Chem. High Thr. Scr., 2011
- Curr. Protein Prop. Sci., 2007
- J. Chem. Inf. Model., 2015
- J. Struct. Biol., 2014
- J. Chem. Inf. Model., 2012
- Bioorg. Med. Chem., 2010
- Bioorg. Med. Chem., 2010
- Bioorg. Med. Chem., 2010
- Phys. Chem. A., 2009
- J. Biol. Struct. Des., 2013
- Chem. Eur. J., 2012
- J. Phys. Chem. C., 2011
- J. Mol. Catal. A: Chem., 2012
- Theor. Chem. Acc., 2012
- J. Phys. Chem. Lett., 2011
- Int. J. Quant. Chem., 2011
- J. Phys. Chem. A., 2010
- Chem., 2010
- Int. J. Quant. Chem., 2010
- Tet. Lett., 2009
- Comput., 2008
- Bioorg. Med. Chem. Lett., 2007
- J. Comput. Chem., 2007
- J. Heterocyclic Chem., 2006
- Rapid Commun. Mass Spectrom., 2007
- Rapid Commun. Mass Spectrom., 2007
- Met. BioSci., 2016
- Med. Chem., 2012
- Comput.-Aided Drug Des., 2012
- Med. Chem. Res., 2012
- J. Mol. Model., 2011
- Org. Med. Chem. Lett., 2011
- J. Heterocyclic Chem., 2006
- Rapid Commun. Mass Spectrom., 2007
- Comp. Pharma. Design., 2008
- Eur. J. Med. Chem., 2008
- J. Mol. Graph. and Model., 2007
- J. Comput. Aided Med. Des., 2007
- QSAR & Comb. Sci., 2006
- Tet. Lett., 2006
- Modeling P450-catalyzed reactions
- Bioorg. Med. Chem., 2017
- J. Am. Chem. Soc., 2010
- Chem. Eur. J., 2011
- J. Phys. Chem. A., 2012
- J. Phys. Chem. B., 2012
- J. Comput.-Aided Med. Des., 2006
- Struct. Chem., 2013
- J. Phys. Chem. A., 2011
- J. Phys. Chem. A., 2011
- Chem. Commun., 2011
- Euro. J. Med. Chem., 2010
- J. Chem. Theory, 2009
- Tet. Lett., 2007
- Int. J. Quant. Chem., 2007

Selected Activities @ CSIR - NEIST

- Dr. Binyo K. Saikia, CSIR - NEIST Received SSB prize
- Established the Regional cum Facilitation Center (RCFC)
- Established of Centre for Infectious Diseases
- Established Centre of Excellence in Advanced Computation and Data Sciences
- Established Centre for Petroleum Research
- INSACOG has recognised CSIR-NEIST as the premier facility centre in North-East

New Initiatives and Technologies

- Healthcare: Antibiotics, PUNGE-DASHRUP
- Vector Control: Mos Care, Mos Eggs
- MSME Scale
- Aroma Mission
- Floriculture
- Honey
- STINER
- BIONEST
- Eco Friendly Campus
- CoE Petroleum Research
- COVID Testing lab
- Genome Sequencing
- Artificial Intelligence
- Immunity Mission
- Coal Research
- CoE Advanced Computation

CSIR-Summer Research Training Program (CSIR-SRTP): The Entire Story

CSIR-SRTP 2020

- 16,394 participants
- 533 sessions
- 68,480 hand-on sessions
- 234 videos
- 236 YouTube subscribers

Drug Discovery Hackathon 2020 Training Program

- Vertical 1: Focused on the theory and computational methods
- Vertical 2: Focused on algorithm and methods development
- Vertical 3: Hands-on sessions on open source and commercial software

Strengthening the computational drug discovery in India

- July 13 - 11: 38 Lectures 18 hand-on session
- August 1 - 30: 38 Lectures 18 hand-on session
- Sept 1 - 11: 18 Lectures 11 hand-on session
- 84 Lectures
- 64 Hands on sessions