

## Bio-data

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1. **Name:** Prof. Ravishankar Ramachandran

2. **Date of Birth:** 2nd July 1970

3. **Current position and Address:**

Chairperson, Biochemistry & Structural Biology Division  
Chief Scientist, CSIR-Central Drug Research Institute,  
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4. **Educational Qualifications**

Sl. No.	Degree/Certificate	Year of passing	University/ Institute	Subjects
1.	Ph.D	1999	Indian Institute of Science, Bangalore	Molecular Biophysics/ Structural Biology
2.	M.Sc	1992	Sri Sathya Sai Institute of Higher Learning	Physics
3.	B.Sc	1991	Sri Sathya Sai Institute of Higher Learning	Physics, Chemistry, Maths

5. **Academic/ Research experience/ Employment**

Sl. No.	From	To	Name of Organization	Position held
1.	12-12-2011	present	CSIR-Central Drug Research Institute	Head, BSB division & Chief Scientist
2.	12-12-2011	12-12-2016	CSIR-Central Drug Research Institute	Senior Principal Scientist
3.	12-12-2006	12-12-2011	-do-	Principal Scientist
4.	12-12-2002	12-12-2006	-do-	Senior Scientist

5.	1999	2002	Max-Planck Institute for Biochemistry, Martinsreid, Germany	Alexander von Humboldt fellow, Nobel laureate Prof. Robert Huber's lab
6.	1993	1999	Indian Institute of Science, Bangalore	Ph.D fellow, Prof. M. Vijayan's lab, Molecular Biophysics Unit

## 6. Honors/Awards received

- *National Bioscience Award for Career Development, 2010*, by the Department of Biotechnology, Ministry of Science & Technology, Govt. of India
- *NASI-SCOPUS Young Scientist Award, 2010*, by the National Academy of Sciences, Allahabad, India & M/s Elsevier.
- *Alexander von Humboldt fellow*
- *Incentive Award for Technology, 2021, CSIR-CDRI, for 'Process for the preparation of Umifenovir (Antiviral)'*
- vLife Best Publication Award, 2013, in recognition of outstanding publication in the field of Computer Aided Drug and Molecular Design.
- Eli-Lilly Certificate of Appreciation for '*Thesis Advisor for 2009 Eli Lilly and Company Asia Outstanding Thesis Awardee*'.
- *Prof. M.P. Khare memorial lecture award*, 20<sup>th</sup> Feb'08, Chemistry department, Lucknow University
- *Plenary speaker*, 25<sup>th</sup> Jan'08, International Molecular Symposium, Chonnam National University, Gwangju, Republic of Korea
- *Max-Planck-Institute fellowship*

## 7. Professional Affiliations

- Member, Academic planning and Development committee (APDC) of NIPER-Hajipur (<http://www.niperhajipur.ac.in>), June, 2020 onwards
- Member, Task Force on Repurposing of Drugs for COVID19, Constituted by Principal Scientific Advisor to the GoI, as part of S&T Core Group on COVID19, (<https://nclinnovations.org/covid19/>), April 2020 onwards.
- Member, Ethical committee, ERA's Lucknow Medical College and Hospital, September 2021 onwards
- *Indian Crystallographic Association*, (<http://iris.physics.iisc.ernet.in/ica/>), Life member (LM 449), 2012, Joint secretary and Executive body member, Nov'13 -June-2016.
- *The Society of Biological Chemists, India*, (<http://sbcihq.in>), Life member (No. 4349), 31/09/2020
- *Indian Society of Cell Biology*, (<http://www.iscb.org.in/>), Life member (No. 5451), 07/09/2012
- *Bioinformatics and Drug Discovery Society*, (<https://www.bidds.org/>), Life member (BIDDS17-40), 10<sup>th</sup> Nov'2017 onwards
- Working group on new TB drugs(WGND),(<http://www.newtbdrugs.org/members.php>), member, 2012
- Member and PI of the core-committee for a National DBT project(s) to enable access at *European Synchrotron Radiation Facility*, Grenoble, France to the Indian scientific community, 2008- 2016
- Member and PI of the committee to enable access to the small-angle X-ray scattering and X-ray crystallography beamlines at European Synchrotron Radiation Facility (ESRF) -2016 onwards

- DBT nominee, Institutional Biosafety Committee, Balasaheb Bhimrao Ambedkar University (BBAU), 2016 onwards
- DBT nominee, Institutional Biosafety Committee, CSIR-Indian Institute of Toxicological Research, 2013 onwards

## 9. List of Patents:

### i) applied/filed for:

Se. No.	TITLE	INVENTOR(S)	Country	APPLICATION NUMBER	COMPLETE/ Provisional FILING DATE
1	Combination of Clofazimine and Imatinib for effective therapy of drug-resistant myeloid leukemia	Sabyasachi Sanyal, Harish Kumar, Naibedya Chattopadhyay, <b>Ravishankar Ramachandran</b> , Arun Kumar Trivedi, Sonal Shree, Anagha Ashok Gurjar, Sourav Chattopadhyay, Sapana Kushwaha, Abhishek Kumar Singh, Shikha Dubey, Kiran Lata, Riyazuddin Mohammed, Jiaur Raha	India	201711030707	24-Aug-18
2	Peptide inhibitors as novel anti-hiv therapeutics	Raj Kamal Tripathi, Balwant kumar, <b>Ravishankar Ramachandran</b> , Jitendra Kumar Tripathi, Smrati Bhadauria & Jimut Kanti Ghosh	India	0594DEL2012	04-Mar-13
3	Novel 4-nitrobutanoates, their acid derivatives and salts thereof	Ranjana Srivastava, Brahm Shanker Srivastava, Manish Kumar Gupta, Rama Pati Tripathi, Neetu Tiwari, Diksha Katiyar & <b>Ravishankar Ramachandran</b>	India	0671DEL2006	07-Dec-06 (Enquiry in 2018)
4	Novel glycosyl ureides useful as inhibitors of NAD+ DNA ligase from M. tuberculosis	Rama Pati Tripathi, Neetu Tiwari, Sandeep Srivastava & <b>Ravishankar Ramachandran</b>	India	0610DEL2006	08-Mar-06
5	New SMAC mimetics for cancer therapy	Haq W, Ali R, Singh A, Nengroo MA, Katekar R, Singh G, Vaishnav J,	India	202011055682	2021

		Afsar M, Singh M, Rath SK, Koley D, Mishra DP, <b>Ravishankar Ramachandran</b> , Ampapathi RS, Gayen JR, Datta D.			
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ii) granted:

S e. N o.	TITLE	INVENTOR(S)	Coun try	APPLI CATIO N NUMB ER	COMPL ETE/ Provisio nal FILING DATE	PATE NT NUMB ER	DAT E OF GRA NT
6.	Novel dispiro cycloalkanones as inhibitors of NAD <sup>+</sup> - dependent DNA Ligase and antitubular agents	Rama Pati Tripathi, Jyoti Pandey, Nimisha Singh, Divya Dubey, Vandana Kukshal, Shalini Bhatnagar, Sudhir Sinha, Vinita Chaturvedi & <b>Ravishankar Ramachandran</b>	India	0182D EL2010	17-Jan-11	29435 4	15-Mar-18
7.	Combination of Clofazimine and Imatinib for effective therapy of drug-resistant myeloid leukemia	Sabyasachi sanyal, Harish kumar, Naibedya chattopadhyay, <b>Ravishankar Ramachandran</b> , Arun kumarv trivedi, Sonal shree, Anagha ashok gurjar, Sourav chattopadhyay, Sapana kushwaha, Abhishek kumar singh, Shikha dubey, Kiran lata, Riyazuddin mohammed, Jiaur rahman	Unite d States	16/117 156		US105 76078 B2	Grant ed on 03- 03- 2020
8.	Peptide inhibitors as novel anti-HIV therapeutics	Raj Kamal Tripathi, Balwant kumar, <b>Ravishankar Ramachandran</b> , Jitendra Kumar Tripathi, Smrati	Unite d States (Thro ugh PCT)	14/382 428 (PCT/IB 2013/0 51641)	02-Sep-14 (01-Mar-13)	93270 09 (USA 14382 428)	03-May-16

		Bhadauria & Jimut Kanti Ghosh					
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#### 10. Mentorship provided (Students guided, teaching etc.):

The author has guided the Ph.D thesis of 17 students. About 7 students are presently working under his guidance for their Ph.D, 1 post graduate thesis student, and post graduate Project assistant-II. Additionally, a 'Nehru-scheme' faculty was mentored by him.

S. N.	Name of PhD students	Thesis title	Year of completion
1	Dr. Sandeep Kumar Srivastava	Structural studies on NAD <sup>+</sup> -dependent DNA ligase (Rv3014c) from <i>Mycobacterium tuberculosis</i> H37Rv	2005
2	Dr. Sarvind Mani Tripathi	Structural studies on latent phase metabolic pathway protein(s) from <i>Mycobacterium tuberculosis</i> H37Rv	2008
3	Dr. Tripti Shrivastava	Structural studies on transcriptional regulatory and metabolic protein(s) from <i>Mycobacterium tuberculosis</i> H37Rv	2008
4	Dr. Amit Luthra	Structural studies on hypothetical protein(s) from <i>Mycobacterium tuberculosis</i> H37Rv	2008
5	Dr. Shuja Shafi Malik	Structural studies on transcriptional regulatory protein(s) from <i>Mycobacterium tuberculosis</i> H37Rv	2008
6	Dr. Gauri Misra	Structural studies on protein(s) involved in transit peptide mediated transport in <i>Plasmodium falciparum</i>	2009
7	Dr. Divya Dube	Identification and optimization of novel inhibitors against proteinaceous drug targets from pathogenic species using <i>in silico</i> approaches	2009
8	Dr. Gaya Prasad Yadav	Structural and functional studies on molecules of biological importance	2010
9	Dr. Vandna Kukshal	Structural and functional characterization of eubacterial DNA ligases	2011
10	Dr. Abhishek Dey	Structural studies on transcriptional regulatory protein(s) from <i>Mycobacteria</i>	2014
11	Dr. Amit Gaur	Structural and functional studies of protein(s) involved in secretion pathways of <i>Mycobacteria</i>	2014

12	Dr. Taran Khanam	Structural and functional studies on protein(s) from human pathogens involved in nucleic acid metabolism	2014
13	Dr. Aparna Agrawal	Structural and functional characterization of transcription regulatory protein(s) from <i>Mycobacterium tuberculosis</i> and <i>BmTPP</i>	2015
14	Dr. Sonal Shree	Structural and Functional Studies on ACT/ RAM domain containing Protein(s) from Mycobacteria	2016
15	Dr. Kiran Lata	Molecular Mechanisms of Mycobacterial proteins involved in nucleic acid metabolism	2018
16	Dr. Ankita Shukla	Structural and functional characterization of protein(s) involved in mycobacterial DNA repair	2020
17	Dr. Mohammad Afsar	Structural and functional characterization of protein(s) involved in nucleic acid metabolism in Mycobacteria	2021
18	Shikha Dubey	Structural and functional studies of selected regulatory and metabolic proteins of <i>Mycobacterium tuberculosis</i>	2021
19	Vijay Kumar Sharma	Structural and functional characterization of protein(s) from the ESX /Type VII secretion pathway	2021

### Post-graduation thesis

Every year, the author guides about 1 student for his/her Post graduate thesis (6 months) and/or postgraduate training on advanced techniques in biotechnology, structural biochemistry, X-ray crystallography, computational biology, protein purification and characterization every year. Totally more than 20 students have been guided for the same.

### 11. Selected invited lectures of the author

- Chief Guest, World Pharmacy day celebrations, 'Story of Umifenovir, a drug repurposing Phase III trial against COVID-19', Babu Sunder Singh College of Pharmacy, Lucknow, 25<sup>th</sup> Sept' 2021
- Invited speaker, Title "BERosomes: Characterisation and development of novel therapeutic approaches" Chemical Biology Society, India, Annual Conference, September 16-17, 2021, Organized Jointly by CBS, CSIR-IICB and NIPER-Kolkata
- Keynote speaker, Title: "Novel functions of an essential Phosphoserine phosphatase involved in Serine metabolism in Mycobacteria", National conference entitled 'Host-pathogen interaction: present and future perspective', 24<sup>th</sup> - 25<sup>th</sup> Sept. 2020 at Department of Life Science, NIT Rourkela, Odisha
- Keynote speaker, Title: "Rational strategies in early target discovery and drug development", National E-Seminar on 'Computational to Lab Strategies for COVID-19' and Amity Institute of Biotechnology, AUUP-Lucknow Campus, 29-30<sup>th</sup> June 2020
- Chief guest and Inaugural lecture, Title: "Early target discovery, Disease biology, and Discovery of new therapeutic avenues against drug-resistant bacteria/ TB", National Seminar on Application of Bioengineering and Bioinformatics in Healthcare", 18<sup>th</sup> February, 2020, Amity University, Lucknow
- Plenary lecture, Title: "Characterization of DNA Base Excision Repair complexes: Implications for new therapeutic strategies", Regional Centre for Biotechnology,

International Workshop & Symposium titled "Structure assisted discovery of novel therapeutics, 15th Feb 2019

- DNA Base Excision Repair in Mycobacteria: A Target for New Therapeutic Development, Invited lecture, International symposium on Advances in Functional and Biological Materials (ISAFBM-2019), 28th Feb 2019, organized by Humboldt Academy, Lucknow
- Exploiting Molecular mechanisms in the DNA Base Excision Repair (BER) pathway
- as a new therapeutic approach against Anti-microbial resistance, Amity University, 26th Feb 2019
- Invited lecture, Hands-on workshop, "Recent advances in Genomics and Proteomics, 5th March 2019 at Bansal Institute of Engineering and Technology, Lucknow
- Plenary lecture, 'Architecture and molecular mechanism of multi-protein complexes (BERosomes) involved in DNA Base Excision Repair (BER)' 46th National Seminar on Crystallography, NIMHANS, Bengaluru, 29<sup>th</sup> June 2018
- Invited lecture, National Seminar on, "Key aspects of Interface between Biology and Engineering", 18th Oct, 2016, Amity University, Lucknow, Title: "Exploitation of X-ray instrumentation technology for protein structure determination and new inhibitor discovery"
- Panel Expert and Nominated Lecture, "Workshop on Bio-Entrepreneurship and Bio-Enterprise creation", by National Academy of Sciences, India, and Biotech Consortium India Ltd., New Delhi, 16th Sept'16, at Biotech Park, Lucknow
- Invited lecture, Workshop on "Recent Trends in Bioinformatics and Computational Biology: An Introduction", Biotech Park, Lucknow, 8th Sept'16. Title: "Structural biology and its applications in drug discovery"
- Invited lectures (2 Nos.), "Structural Biology and its Application in Drug Discovery", Amity University, Lucknow, 6th Sept'16
- Invited lecture, 'National Seminar on Crystallography (NSC44), IISER Pune, 10th July'16, Title: 'Enlisting RAM in the fight against tuberculosis'
- Invited Lecture, Workshop on "In-Silico Strategies for Disease Pathway Analysis & Biomarker Discovery" from March 29 – 31, 2016
- Keynote lecture & Chief guest, 'Workshop on DNA analytics using Java', 29th March 2016, Amity University, Lucknow. "DNA interacting proteins from M. tuberculosis"
- Invited lecture in CCMB, Hyderabad, 21st May 2015, Title: 'A novel tri-component DNA Base-excision repair (BER) complex in Mycobacterium tuberculosis'
- Invited lecture in ' XXXVIII All India Cell Biology Conference & Symposium, 10-12th Dec'14 Title: 'Characterisation of a haloaciddehalogenase from M. tuberculosis that has invasion-like properties'
- Chaired a session in the International conference titled "Frontiers in Structural Biology: New Advances in X-ray Diffraction and Cryo-electron Microscopy" held between 15th-17th Dec' 2014. at INSA New Delhi
- Talk in International Symposium: "Crystallography in Physics, Chemistry and Biology"; 3rd Mar'14, Title: "Mycobacterial DNA Base Excision Repair and New inhibitor strategies", CSIR-CDRI, Lucknow
- Lectures at 'Beijing genomics institute'/ Shanghai, China, 21/10/ - 02/11, 2003
- Plenary speaker, 'International Symposium of Molecular Science', Chonnam National University, Gwangju, Korea, 25/01/08
- International workshop on application of X-ray diffraction for Drug Discovery' JNU, New Delhi, 23rd Nov'13, 'Towards discovery of anti-TB inhibitors that: Target components of the BER pathway and those responsible for the adaptation/maintenance of TB persistence'



- Emerging themes in Tuberculosis Research, IISc, Bangalore, 20th July'13 'Towards the discovery of TB inhibitors'
- Invited lecture at Amity University, Lucknow, 21st Feb'14, Structural Biology: New Research Aspects
- Prof. M.P. Khare memorial lecture, 20th Feb' 08, Chemistry department, Lucknow University
- Invited guest and speaker at the Annual day celebrations of 'CSIR-CIMAP, 26th Mar'12, on 'Structural Biology: understanding molecular mechanisms of proteins and applications to new inhibitor discovery'.
- Invited lecture on 'Structural biology approaches to drug discovery', Humboldt academy and Physics department, Lucknow University, 13/02/08
- Invited lecture: Macromolecules-Structure and function, 80th Society of Biological Chemists (SBC) meeting, 13/11/11
- Invited lecture in Banaras Hindu University, 14th Feb'10, on 'Understanding the molecular mechanisms of proteins from human pathogens using structural biology - Identification of novel inhibitors with therapeutic potential using rational approaches'
- Invited lecture, King George's Medical University, 23rd July'10, 'Structural biology and its application to the rational design of inhibitors,
- CDRI-Niper symposium, 26th Mar'10, 'Novel structural weapons to fight Tuberculosis',
- Symposium on 'Current advances in biological research', CSIR-Indian Institute of Toxicological Research, 2nd Feb'09
- Workshop on ' Structural biology and applications to drug discovery' organized by the author, 30th Oct'09
- 'Structural biology aspects', Amity University, 6th Mar'13
- Regularly delivers about 2 invited lectures a year in the DBT-workshops on bioinformatics and rational drug discovery' organized by Biotech park, Lucknow from 2003-04 onwards

## 12. Technologies Developed/Transferred:

(a) Number of Technologies developed:

Se. No.	Technologies developed	Remarks
1.	<b>Drug-targets for Dyslipidemia, drug-resistant TB &amp; Filariasis</b> The author <u>has secured the Artificial Intelligence Molecular Screen (AIMS) Award by M/s Atomwise</u> for academic researchers seeking novel compounds to treat disease and is partnering with M/s AtomWise Inc,for development. The specialist team of the company has selected drug 5 targets from the author's group for further <u>multi-target Artificial Intelligence driven drug discovery studies</u> . The targets are in the disease areas of Dyslipidemia, drug-resistant TB & Filariasis.	The targets: human PCSK9, Sliding $\beta$ -clamp (aka DnaN), Lysine- $\epsilon$ aminotransferase, Trehalose 6-phosphate phosphatase, and HGPRT have been selected for <b>AIMS Awards of M/s Atomwise Inc.</b>



2.	<b>SerB2 is a target for multi-drug-resistant TB:</b> The author has demonstrated that the essential SerB2, involved in mycobacterial Serine metabolism is exported and interacts with human host factors. He has identified that it is a target for Clofazimine, a drug that is being evaluated clinically against MDR- and XDR-TB and also for Chlorpromazine. The technology is for <u>drug-repositioning against multi-drug-resistant TB infection</u> .	<b>An agreement has been signed with the Global TB Alliance</b> ( <a href="https://www.tballiance.org/about/mission">https://www.tballiance.org/about/mission</a> ) for evaluation of related Riminophenazines and other molecules against this target.
3.	<b>Drug repurposing against Imatinib-resistant Chronic Myeloid Leukemia (CML):</b> Our team <u>identified a candidate drug (Clofazimine) for repurposing against chronic myeloid leukemia</u> . The drug acts through a novel mechanism in this disease and is targeted for patients with Imatinib-resistant CML	<b>-Phase II clinical trials being planned/ filed for</b> -US patent already secured (US10576078B2)
4.	<b>Shikimate Kinase as the target for Rottlerin:</b> we identified that Rottlerin a known anticancer inhibitor targets Shikimate kinase of Mtb to effect anti-TB activity paving the way to exploit this novel target using this scaffold	<b>Commercial/ Industry co-development partners being identified</b>
5.	<b>Inhibitors to disrupt HIV-1 Nef-co-protein interactions</b> The author's leading work as part of a team identified inhibitors to disrupt HIV-1 Nef-co-protein interactions like those with ASK-1. He solved the crystal structure of HIV-1 full-length Nef based on patient's sequence and identified new inhibitors. This technology development of anti-HIV therapeutics with new modes of action is available and can be targeted against latent viral reserves. The efforts have been protected by US patent/ PCT patent	<b>Commercialization/ co- development Industrial partners are being identified</b>

(b) Number of Technologies transferred/ commercialized to industry

Se. No.	Technology	Industry
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1.	<b>Detailed method of preparation of antiviral molecule, Umifenovir:</b> process monitoring along with process control method, Specifications of raw materials used in the synthesis and specifications and test procedures of the finished product. <i>The author is the Nodal PI for the team</i>	<b>M/s Medizest Pharmaceuticals Pvt. Ltd., Goa</b> 24/04/2020
2	<b>Phase III clinical trials</b> MOU signed between CSIR-CDRI and M/s MARC laboratories, Lucknow for conducting Phase III clinical trials on Niclosamide against COVID19 caused by Sars Cov2 <i>The author is the Nodal PI for the team</i>	<b>M/s Marc Laboratories Ltd., Lucknow,</b> 18/08/2020

(c) Clinical Trials

Se. No.	Technology	Industry partner
1.	<b>DCGI approved “Phase 3, Randomized, Double-blind, Placebo control trial of Efficacy, Safety and Tolerability of Antiviral drug Umifenovir vs Standard care of therapy in non-severe COVID-19 patients”</b>  <i>The author is the Nodal PI for the clinical trials</i>	Trial completed by CSIR-CDRI and M/s Medizest Pharmaceuticals Pvt. Ltd., Goa

### 13. Brief summary of key research contributions

Ravishankar secured Ph.D from Indian Institute of Science, Bangalore and subsequently carried out excellent work at Max-Planck Institute for Biochemistry as a Humboldt Fellow with Prof. Robert Huber, a Nobel laureate. He returned to India in 2002 to start an independent research group at CSIR-Central Drug Research Institute, Lucknow.

Ravishankar has made outstanding contributions in the areas of disease biology of TB infection and designing of therapeutic molecules, especially to understand the molecular basis of ‘Feast/ famine regulation’ and ‘DNA Base-Excision-Repair (BER)’ that are critical for the pathogen. He has elegantly used Structural biology, Rational drug-discovery and Drug-target based approaches to identify novel inhibitors with therapeutic potential that target these pathways and to overcome Anti-microbial drug-resistance. His contributions have brought International recognition and National awards like the *National Bioscience Award for Career Development*, 2010, by the Department of Biotechnology, Ministry of Science & Technology, Govt. of India & *NASI-SCOPUS Young Scientist Award*, 2010, by the National Academy of Sciences, Allahabad, India & M/s Elsevier.

Very recently, Ravishankar led a team that successfully completed “*Phase III, Randomized, Double-blind, Placebo controlled trial of Efficacy, Safety and Tolerability of Antiviral drug Umifenovir vs Standard care of therapy in non-severe COVID-19 patients*” conducted by CSIR-CDRI in association with three renowned medical university/ hospitals located in Lucknow, India,

involving a total of 123 patients. Commercialization of the same is in advanced stages and a patent to protect the dosage used in the study is being filed internationally.

Some of his major contributions are detailed below:

(a) Characterization of BEROsomes in Mycobacteria and novel therapeutic strategies:

BEROsomes are large multi-molecular complexes that function in the DNA Base Excision repair (BER) pathway. Ravishankar's group has pioneered the study of several such BEROsomes from Mtb and has identified multiple scaffolds that disrupt BEROsomes and/or target novel target sites. These include his studies on DnaN (sliding  $\beta$ -clamp)-class II apurinic/apyrimidinic-endonuclease/3'-5' exonuclease (XthA) in the presence and absence of DNA substrate, XthA-NAD<sup>+</sup>-dependent DNA Ligase A, Nei2-DnaN, and others. He has dissected the molecular mechanisms of the individual components and the respective BEROsomes to identify novel therapeutic strategies that involve either disrupting the multimeric assemblies or by strengthening them to block the pathway. His studies have led to the identification of new classes of compounds that exhibit anti-bacterial specificity and distinguish the human enzyme several fold, both *in vitro* and in LigA-deficient strains. More recently he showed that XthA engages with LigA to form a BEROsome whose function is to counter futile cleavage and ligation cycles in Base Excision Repair. The latter represents a fundamental Base Excision Repair interaction that is necessary for effective and critical repair of damaged DNA. Disrupting this process can lead to new therapeutics for drug resistant bacteria/mycobacteria that have less toxic side-effects.

(b) Discovered that Mtb SerB2 is a target for Clofazimine against MDR and XDR-TB:

Ravishankar has identified new functions for an essential mycobacterial HAD phosphatase (SerB2). Using Broncho Alveolar Lavage (BAL) samples from TB patients, he showed that it is secreted and mediates host-pathogen interactions. He subsequently identified several small-molecule inhibitors for it, including Clofazimine that is being evaluated in clinical trials against drug resistant TB by the Global TB alliance. The results excitingly demonstrate that SerB2 is a target for riminophenazines being evaluated clinically. A translational output in this context is that an agreement with the 'Global TB Alliance' was signed by his group/ CDRI for evaluating such compounds.

(c) Molecular mechanisms underlying Feast-Famine regulation in mycobacteria:

Feast/famine regulatory proteins (FFRPs) are global regulators that apparently help mycobacteria to switch/ adapt from 'Feast' to 'Famine' state. Ravishankar's studies importantly suggest how mycobacterial FFRPs can form nucleosome-like particles, and how effector-binding events can trigger specific regulatory outcomes. First-in-class small-molecule inhibitors have been identified by his group against an FFRP. He has also demonstrated that the rarely observed 'open' quaternary association is an operating principle in these regulators, that otherwise adopt closed oligomeric symmetry. The 'open' quaternary structure is important for the protein to bind to non-symmetric target DNA sites, and can be triggered in response to changes to the effector binding site; eg. those that occur upon ligand binding for regulatory activities.

- (d) Direct evidence for a glutamate 'switch' mechanism has been identified to operate in a sub-class of aminotransferases, and carried out associated structure-function studies on mycobacterial factors like Lysine  $\epsilon$ -aminotransferase (MtbLAT) and L-Alanine dehydrogenase (MtbALD) that are thought to be important for adaptation/maintenance of tuberculosis persistence/latency. The latter have incidentally been ranked among the top-3 targets against tuberculosis persistence by the TB-Structural-Genomics Consortium. The results were exploited to identify the very first inhibitors of MtbLAT using structure-based approaches that promise to be useful against persistent TB-infection.
- (e) Drug Repurposing of Umifenovir against Sars-Cov2. Ravishankar led a team that conducted the first *"Phase III, Randomized, Double-blind, Placebo controlled trial of Efficacy, Safety and Tolerability of Antiviral drug Umifenovir vs Standard care of therapy in non-severe COVID-19 patients"* in association with three renowned medical university/hospitals located in Lucknow, India, involving a total of 123 patients. The Phase III trial represents the first double-blind placebo controlled trial to evaluate Umifenovir against COVID-19. The drug Umifenovir was identified and shortlisted based on the efficacy, toxicity, patent status and other favourable parameters. The interactions with COVID19 target was evaluated in vitro and computationally. Since it is not available in India, the process was implemented and transferred to a company (M/s Medizest, Goa) for manufacture under GMP conditions. Careful analysis of the dosage needed for COVID19 patients was carried out based on the reported pharmacokinetics. The results of the Phase III trial support the use of Umifenovir in Mild-asymptomatic COVID-19 patients. Commercialization is at an advanced stage. PCT and Indian patents to protect the dosage used is being filed.

## Complete Publication list of Dr. Ravishankar Ramachandran

1. Banerjee, R., Das, K., **Ravishankar Ramachandran**, Suguna, K., Surolia, A. & Vijayan, M. (1996). Conformation, protein-carbohydrate interactions and a novel subunit association in the refined structure of peanut lectin-lactose complex. *J. Mol. Biol.*, 259, 281-296.
2. **Ravishankar Ramachandran**, Ravindran, M., Suguna, K., Surolia A. & Vijayan, M. (1996). Crystal structure of the Peanut lectin-T-antigen complex. *Prog.Biophys. Mol. Biol.* 65 Suppl. 1, 33.
3. **Ravishankar Ramachandran**, Ravindran, M., Suguna, K., Surolia A. & Vijayan, M. (1997). Crystal structure of the peanut lectin-T-antigen complex. Carbohydrate specificity generated by water bridges. *Current Science* 72, 855-861. (also: *Current Science*, (1999) 76, 1393)
4. **Ravishankar Ramachandran** Nagasuma Chandra, R. & Vijayan M. (1998). X-ray studies on crystalline complexes involving amino-acids and peptides XXXIV. Novel mode of aggregation, Interaction patterns and chiral effects in the maleic acid complexes of DL- and L-Arginine. *J. Biomol. Struc. Dyn.* 15, 1093-1100.
5. **Ravishankar Ramachandran** Surolia, A., Vijayan, M., Lim, S. & Kishi, Y. (1998). Preferred conformation of C-lactose at the free and peanut lectin bound states. *J. Am. Chem. Soc.* 120, 11297-11303.  
(started a flurry of activity in the area of synthetic sugar-protein interactions)
6. **Ravishankar Ramachandran**, Bidya Sagar, M., Roy, S., Purnapatre, K., Handa, P., Varshney, U. & Vijayan, M. (1998). X-ray analysis of a complex of *Escherichia coli* Uracil DNA Glycosylase (EcUDG) with a proteinaceous inhibitor. The structure elucidation of a prokaryotic UDG. *Nucleic.Acids Res.* 26, 4880-4887.  
(with picture in the cover)
7. **Ravishankar Ramachandran**, Suguna, K., Surolia, A. & Vijayan, M. (1999). The crystal structures of the complexes of peanut lectin with Methyl- $\alpha$ -galactose and N-acetyllactosamine and a comparative study of carbohydrate binding in Gal/GalNAc specific legume lectins. *Acta Cryst.D*55, 1375-1382.  
(was cited in the IUCR newsletter (vol. 7 number 3) as one of the important contributions to the field)
8. Bidya Sagar, M., **Ravishankar Ramachandran**, Saikrishnan, K., Purnapatre, K., Handa, P., Varshney, U. & Vijayan, M. (1999). Structural analysis of wild type *E. Coli* Uracil DNA glycosylase (EcUDG) and new crystal forms of its complex with a proteinaceous inhibitor, Ugi. *J. Biosci.*, 24 (supplement 1), 36.
9. **Ravishankar Ramachandran** Suguna, K., Surolia, A & Vijayan, M. (1999). A comparative study of carbohydrate binding in Gal/GalNAc specific legume lectins. *J. Biosci.* 24 (supplement 1), 35.

10. Pratap, J.V., **Ravishankar Ramachandran** & Vijayan, M. (2000). X-ray studies on crystalline complexes involving amino acids and peptides. XXXV. Invariance and variability in amino acid aggregation in the complexes of maleic acid with L- histidine and L- lysine. *Acta Cryst. Sect. B.* B56, 690-696.
11. Song, H.K., Hartmann, C., **Ravishankar Ramachandran** \*, Bochtler, M., Behrendt, R., Moroder, L. & Huber R. (2000) Mutational studies on HslU and its docking mode with HslV. *Proc. Natl. Acad. Sci. (USA)* 97, 14103-14108.  
\*joint first-authors
12. Bochtler, M., Hartmann, C., Song, H.K., **Ravishankar Ramachandran** & Huber R (2000). Docking of components in a bacterial complex. *Nature* 408, 668.  
(see also *Nature* 409 (2001) 152)
13. **Ravishankar Ramachandran**, Thomas, C.J., Suguna, K., Surolia, A. & Vijayan, M. (2001) Crystal structures of the Peanut lectin - lactose complex at acidic pH: Retention of unusual quaternary structure, empty and carbohydrate bound combining sites, molecular mimicry and crystal packing directed by interactions at the combining site. *Proteins: Structure, Function, and Genetics* 43, 260-270.
14. Adhikari P, Bachhawat-Sikder, K, Thomas, C.J., **Ravishankar Ramachandran**, Jeyaprakash, A.A., Sharma, V, Vijayan, M. & Surolia, A (2001). Mutational analysis at N41 in Peanut Agglutinin (PNA): A residue critical for the binding of the Tumor-associated Thomsen-Friedenreich Antigen  
*J. Biol. Chem.* 276, 40734-40739.
15. Bochtler, M., Song, H.K., Hartmann, C., **Ravishankar Ramachandran** & Huber, R (2001) The quaternary arrangement of HslU and HslV in a co-crystal  
*J. Struct. Biol.* 135, 281-293.
16. **Ravishankar Ramachandran**, Hartmann, C., Song, H.K., Huber, R. & Bochtler, M. (2002) Functional interactions of HslV (ClpQ) with the ATPase HslU (ClpY)  
*Proc. Natl. Acad. Sci. (USA)* 99, 7396-7401.
17. Saikrishnan, K., Bidya Sagar, M., **Ravishankar Ramachandran**, Roy, S., Purnapatre, K., Handa, P., Varshney, U. & Vijayan, M. (2002)  
Domain closure and action of uracil DNA glycosylase (UDG). Structures of new crystal forms containing the *Escherichia coli* enzyme and a comparative study of the known structures involving UDG.  
*Acta Crystallogr. D* 58, 1269-1276.
18. Song H.K., Bochtler, M, Azim, M.K., Hartmann, C., Huber, R. & **Ravishankar Ramachandran** (2003). Isolation and characterization of the prokaryotic proteasome homolog HslVU (ClpQY) from *Thermatoga maritima* and the crystal structure of HslV.  
*Biophysical Chemistry* 100, 437-452 (Invited paper in honour of Prof. TS Edsall)
19. M. Kamran Azim, H. K. Song, C. Hartmann, **Ravishankar Ramachandran**, M. Bochtler and R. Huber. (2004). Review: Architecture and assembly of the bacterial HslVU protease complex. *Protein Structure-function relationship. Ed. Ali & Abbasi, Karachi*, 241-252

20. Tripti S., Sandeep K., **Ravishankar Ramachandran** (2004)  
Cloning, expression, purification and crystallization of a transcriptional regulatory protein (rv3291c) from *Mycobacterium tuberculosis* H37rv.  
*Acta Cryst. Section D* 60, 1874-1876
21. Azim, MK, Goehring, W., Song HK, **Ravishankar Ramachandran**, Bochtler M & Goettig P (2005)  
Characterisation of the HslU chaperone affinity for HslV protease  
*Protein Sci.*, **14**, 1357-62
22. Srivastava SK, Tripathi RP, **Ravishankar Ramachandran** (2005)  
NAD<sup>+</sup> -dependent DNA ligase (rv3014c) from *M. tuberculosis*: Crystal structure of the adenylation domain and identification of novel inhibitors.  
*J. Biol. Chem.***280**, 30273-30281
23. Srivastava SK, Dube D, Tewari N, Dwivedi, N, Tripathi RP &**Ravishankar Ramachandran**(2005)  
*Mycobacterium tuberculosis* NAD<sup>+</sup> -dependent DNA ligase is selectively inhibited by glycosylamines compared with human DNA ligase I.  
*Nucleic Acids Res.* **33**, 7090-7101
24. Tripathi SM &**Ravishankar Ramachandran** (2006)  
Over-expression, purification and crystallization of Lysine  $\epsilon$ -aminotransferase (Rv3290c) from *Mycobacterium tuberculosis* H37Rv  
*Acta Crystallogr.* **F62**, 572-575
25. Tripathi, SM &**Ravishankar Ramachandran**(2006)  
Direct evidence for a glutamate switch necessary for substrate recognition: Crystal structures of  
Lysine  $\epsilon$ -aminotransferase (Rv3290c) from *Mycobacterium tuberculosis* H37Rv *J. Mol. Biol.* **362**, 877-886  
(Suggests a common mechanism for a sub-class of aminotransferases)
26. Srivastava SK, Dube D, Vandna, K, Jha AK, Hajela K &**Ravishankar Ramachandran** (2007)  
NAD<sup>+</sup>-dependent DNA ligase (Rv3014c) from *Mycobacterium tuberculosis*: Novel structure-function relationship and identification of a specific inhibitor  
*PROTEINS*:**69**, 97-111
27. Divya Dube, Sandeep Kumar Srivastava, Vandna Kukshal, Rama Pati Tripathi &**Ravishankar Ramachandran** (2007)  
Novel specific inhibitors of NAD<sup>+</sup> -dependent DNA ligase (Rv3014c) identified from virtual screening  
*Med. Chem. Res.***15**, 93
28. Divya Dube, Sarvind Mani Tripathi &**Ravishankar Ramachandran** (2007) Identification of inhibitors of *M. tuberculosis* Lysine  $\epsilon$ -aminotransferase by virtual screening *Med. Chem. Res.***15**, 181



29. Namrata Dwivedi, Divya Dube, Jyoti Pandey, Biswajit Singh, Vandna Kukshal, **Ravishankar Ramachandran\*** & Rama Pati Tripathi\* (2008)  
NAD<sup>+</sup>-dependent DNA ligase: A novel target waiting for the right inhibitor  
*Medicinal Research Reviews* **28**, 545-568, 2008  
\*(Joint corresponding authors)
30. Divya Dube, Vandna Kukshal, Sandeep Kumar Srivastava, Rama Pati Tripathi & **Ravishankar Ramachandran** (2008)  
NAD<sup>+</sup>-dependent DNA ligase (Rv3014c) *M. tuberculosis*: Strategies for inhibitor design  
*Med. Chem. Res.* **17**, 189-198 (In a special Journal issue)
31. Divya Dube, Sarvind Mani Tripathi & **Ravishankar Ramachandran** (2008) Identification of *in vitro* inhibitors of *M. tuberculosis* Lysine  $\epsilon$ -aminotransferase by pharmacophore mapping and three dimensional flexible searches  
*Med. Chem. Res.* **17**, 182-188 (In a special Journal issue)
32. Tripti, S & **Ravishankar Ramachandran** (2007)  
Mechanistic insights from the crystal structures of a feast/famine regulatory protein from *Mycobacterium tuberculosis* H37Rv *Nucleic Acids Res.* **35**, 7324-7335
33. Gauri Misra, Anita Aggarwal, Sonia Mittal, Yogendra Singh & **Ravishankar Ramachandran** (2007)  
Purification, crystallization and preliminary structural analysis of nucleoside diphosphate kinase from *Bacillus anthracis*  
*Acta.Crystallogr. Sect. F* **63**, 1084-1086
34. Tripathi SM & **Ravishankar Ramachandran** (2008)  
Over-expression, purification, crystallization and preliminary X-ray analysis of Rv2780 from *Mycobacterium tuberculosis* H37Rv  
*Acta.Crystallogr. Sect. F* **64**, 367-370
35. Tripathi SM & **Ravishankar Ramachandran** (2008)  
Crystal structures of the *Mycobacterium tuberculosis* secretory antigen Alanine dehydrogenase (Rv2780) in *apo* and ternary complex forms captures 'open' and 'closed' enzyme conformations  
*PROTEINS* **72**, 1089-1095
36. Luthra A, Malik SS & **Ravishankar Ramachandran** (2008)  
Comparative structural analysis of two hypothetical proteins from *Mycobacterium tuberculosis* found in the human granuloma during persistence and highly up-regulated under carbon-starvation conditions  
*Prot. Exp. Purif.* **62**, 64-74
37. Malik SS, Luthra A, Srivastava S & **Ravishankar Ramachandran** (2008)  
The *M. tuberculosis* UsfX (Rv3287c) exhibits novel nucleotide binding and hydrolysis properties  
*Biochem.Biophys. Res. Comm.* **375**, 465-470
38. Luthra A, Mahmood, A, Arora A & **Ravishankar Ramachandran** (2008)  
Characterization of Rv3868: an essential hypothetical protein of the ESX-1 secretion system in *M. tuberculosis*  
*J. Biol. Chem.*, **283**, 36532-36541

39. Malik SS, Luthra A & **Ravishankar Ramachandran** (2009)  
Interactions of the *M. tuberculosis* UspX with the cognate sigma factor SigF and the anti-anti sigma factor RsfA  
*Biochim.Biophys. Acta*, **1794**, 541-553 IF 3.64
40. Misra G, Aggarwal A, Dube D, Zaman MS, Singh Y & **Ravishankar Ramachandran** (2009) Crystal structure of the Bacillus anthracis nucleoside diphosphate kinase and its characterization reveals an enzyme adapted to perform under stress conditions  
*PROTEINS*, **76**, 496-506
41. Jyoti Pandey, Anindra Sharma, Vinod K. Tiwari, Divya Dube, **Ravishankar Ramachandran**, Vinita Chaturvedi, Sudhir K. Sinha, Nripendra N. Mishra, Praveen K. Shukla, Rama P. Tripathi (2009)  
Solution phase synthesis of a library of carbapeptide analogues based on glycosylamino acid scaffolds, their *in silico* screening and antimicrobial evaluation  
*J. Comb. Chem.*, **11**, 422-427 – IF 3.41
42. Misra G & **Ravishankar Ramachandran** (2009)  
Hsp70-1 from Plasmodium falciparum: Protein stability, domain analysis and chaperone activity  
*Biophys. Chem.* **142**, 55-64
43. Tripti Shrivastava, Abhishek Dey & **Ravishankar Ramachandran** (2009)  
Ligand induced structural transitions, mutational analysis and 'open' quaternary structure of the *M. tuberculosis* Feast/famine regulatory protein (Rv3291c)  
*J. Mol. Biol.* **392**, 1007-1019
44. Ramachandran *et al.* (~60 authors), (2009) *Mycobacterium tuberculosis* systems biology data in R *Biobytes* **5**, 40-48
45. Gauri Misra & **Ravishankar Ramachandran** (2010)  
Exploring the positional importance of aromatic residues and lysine in the interactions of peptides with the *Plasmodium falciparum* Hsp70-1  
*Biochim.Biophys.Acta* **1804**, 2146-2152 - IF 3.64
46. Ajay A, Singh V, Singh S, Pandey S, Gunjan S, Dubey D, Sinha SK, Singh BN, Chaturvedi V, Tripathi R, **Ravishankar Ramachandran** & R. P. Tripathi (2010)  
Synthesis and bio-evaluation of alkylaminoaryl phenylcyclopropyl methanones as antitubercular and antimalarial agents.  
*Bioorg. Med. Chem.* **18**, 8289-8301
47. Bhargavan B, Singh D, Gautam AK, Mishra JS, Kumar A, Goel A, Dixit M, Pandey R, Manickavasagam L, Dwivedi SD, Chakravarti B, Jain GK, **Ravishankar Ramachandran**, Maurya R, Trivedi A, Chattopadhyay N & Sanyal S (2012)  
Medicarpin, a Legume Phytoalexin, Stimulates Osteoblast Differentiation and Promotes Peak Bone Mass Achievement in Rats: Evidence for Estrogen Receptor  $\beta$ -mediated Osteogenic Action of Medicarpin.  
*J. Nutr. Biochem.* **23**, 27-38. - IF 4.54
48. **Ravishankar Ramachandran** (2011)

Letter to the Editor: Exploring the positional importance of aromatic residues and lysine in the interactions of peptides with the *Plasmodium falciparum* Hsp70-1  
*Biochim.Biophys.Acta*.**1814**, 457 - IF 3.64

49. Arora A, Chandra, NR, Das A, Gopal B, Mande SC, Prakash B, **Ravishankar Ramachandran**, Sankaranarayanan R, Sekar K, Suguna K, Tyagi AK & Vijayan M (2011)  
Invited review: Structural Biology of *M. tuberculosis* Proteins: The Indian Efforts  
*Tuberculosis (Edinb.)* 91, 456-468. –if 2.65

50. Tripathi RP, Pandey J, Kukshal V, Ajay A, Mishra M, Dube D, Chopra D, Dwivedi D, Chaturvedi V & **Ravishankar Ramachandran** (2011)  
Synthesis, *in silico* screening and bioevaluation of dispiro-cycloalkanones as antitubercular and mycobacterial NAD<sup>+</sup>-dependent DNA ligase inhibitors  
*Med. Chem. Commun.* **2**, 371 – 377

51. Dwivedi SKD, Singh N, Kumari R, Mishra JS, Tripathi S, Banerjee P, Shah P, Kukshal V, Tyagi AM, Chaturvedi RK, Mishra DP, Trivedi AK, Gaikwad AN, Sanyal S, Chattopadhyay N, **Ravishankar Ramachandran**, Siddiqui MI, Bandyopadhyay A, Arora A, Lundåsen T, Priyadarshini AS, Moore DD and Sanyal S (2011)  
Bile Acid Receptor Agonist GW4064 Regulates PPAR $\alpha$  coactivator-1 $\alpha$  Expression through Estrogen Receptor-Related receptor  $\alpha$   
*Mol. Endocrinol.* **25**, 922-932. -IF 5.257

52. Pankaj Singh, Gaya Prasad Yadav, Sudeepti Gupta, Anil Kumar Tripathi, **Ravishankar Ramachandran\*** & **Raj Kamal Tripathi\*** (2011)  
A novel dimer-tetramer transition captured by the crystal structure of HIV-1 Nef (\**Joint corresponding authors*)  
*PLoS ONE* 6(11): e26629. doi:10.1371/journal.pone.0026629 – IF 4.41

53. Deepak Gurbani, Vandna Kukshal, Julian Laubenthal, Ashutosh Kumar, Alok Pandey, Sarita, Ashish Arora, Swatantra K. Jain, **Ravishankar Ramachandran**, Diana Anderson & Alok Dhawan (2012)  
Mechanism of inhibition of the ATPase domain of human topoisomerase IIa by 1,4-benzoquinone, 1,2-naphthoquinone, 1,4-naphthoquinone, and 9,10-phenanthroquinone  
*Toxicological Sciences* 126, 372-390 - IF -5.093

54. Vandna Kukshal, Mridul Mishra, Arya Ajay, Taran Khanam, Rahul Sharma, Divya Dube, Deepti Chopra, Rama Pati Tripathi & **Ravishankar Ramachandran** (2012)  
Synthesis and bioevaluation of aryl hydroxamates distinguishing between NAD<sup>+</sup> and ATP-dependent DNA ligases  
*Med. Chem. Commun.* **3**, 453-461, 2012 (Was specially cited in 'Chemistry World')

55. Vandna Kukshal, Taran Khanam, Deepti Chopra, Nidhi Singh, Sabyasachi Sanyal & **Ravishankar Ramachandran** (2012)  
*M. tuberculosis* sliding  $\beta$ -Clamp does not interact directly with the NAD<sup>+</sup> -dependent DNA ligase  
*PLoS ONE*. 7(4): e35702. doi:10.1371/journal.pone.0035702

56. Kaur J, Dube D, **Ravishankar Ramachandran**, Singh P & Neeloo Singh (2012)  
Thianthrene is a novel inhibitor of the Pteridine Reductase 1 from *Leishmania donovani* clinical Isolate

*J. Mol. Biochem.* **1**, 68-75, 2012

57. Macwan AS, Kukshal V, Srivastava N, Javed S, Kumar A & **Ravishankar Ramachandran** (2012)

Crystal structure of the Hexachlorocyclohexane dehydrochlorinase (LinA-type2): mutational analysis, thermostability & enantioselectivity

*PLoS ONE* 7(11):e50373 doi: 10.1371/journal.pone.0050373

58. Luthra A, Gaur A & **Ravishankar Ramachandran** (2013)

Rv3868 (EccA1), an essential component of the *M. tuberculosis* ESX-1 secretion system, is thermostable

*Biochim. Biophys. Acta* **1834**, 1181-1186

59. Balawant Kumar, Chakrapani Tripathi, Ranjana K Kanchan, Jitendra kumar Tripathi, Jimut K Ghosh, **Ravishankar Ramachandran**, Smrati Bhadauria & Raj Kamal Tripathi (2013)

Dynamics of Physical Interaction between HIV-1 Nef and ASK1: Identifying the Interacting Motifs

*PLoS ONE* 8(6):e67586. doi: 10.1371/journal.pone.0067586.

60. Namrata Anand, K.K.G. Ramkrishna, Munna P. Gupta, Vinita Chaturvedi, Shubhra Singh, Kishore K. Srivastava, Prapunjika Sharma, Niyati Rai, **Ravishankar Ramachandran**, Anil Kumar Dwivedi, Varsha Gupta, Brijesh Kumar, Smriti Pandey, Praveen K. Shukla, Shailandra K. Pandey, Jawahar Lal, & Rama Pati Tripathi (2013)

Identification of 1-[(4-Benzyloxyphenyl)-but-3-enyl]-1H-azoles as New Class of Antitubercular and Antimicrobial Agents

*ACS Med. Chem. Lett.* **4**, 958-963

61. Abhishek Dey, & **Ravishankar Ramachandran** (2014)

Cloning, overexpression, purification and preliminary X-ray analysis of a Feast/famine regulatory protein (Rv2779c) from *Mycobacterium tuberculosis* H37Rv

*Acta Cryst.* **F70**, 97-100

62. Taran Khanam & **Ravishankar Ramachandran** (2014)

Exploiting bacterial DNA repair systems as drug targets: A review of the current scenario with focus on mycobacteria

*J. Indian Institute of Science*, **94**, 149-168

(invited review in IYCR14 celebratory issue of the journal)

63. K. Kumar G. Ramakrishna, Sarika Gunjan, Akhilesh Kumar Shukla, Venkata Reddy Pasam, Vishal M. Balaramnavar, Abhishek Sharma, Swati Jaiswal, Jawahar Lal,

Renu Tripathi, Anubhooti, **Ravishankar Ramachandran**, and Rama Pati Tripathi. (2014)

Identification of Novel Phenyl Butenonyl C-Glycosides with Ureidyl and Sulfonamidyl Moieties as antimalarial Agents

*ACS Med. Chem Lett.*, **5**, 878-883

64. Yadav GP, Sonal Shree, Rai N, Maurya R, Singh DK, Srivastava KK & **Ravishankar Ramachandran** (2014)

Characterization of *M. tuberculosis* SerB2, an essential HAD-family phosphatase, reveals novel properties

*PLoS ONE*. 9(12): e115409. doi: 10.1371/journal.pone.0115409

65. Mohd. Parvez Khan<sup>1§</sup>, Abhishek Kumar Singh<sup>2§</sup>, Amit Arvind Joharapurkar<sup>3</sup>, Manisha Yadav<sup>2</sup>, Sonal Shree<sup>4</sup>, Harish Kumar<sup>2</sup>, Anagha Gurjar<sup>2</sup>, Jay Sharan Mishra<sup>2</sup>, Mahesh Chandra Tiwari<sup>1</sup>, Sudhir Kumar<sup>5</sup>, **Ravishankar Ramachandran**<sup>4</sup>, Anupam Sharan<sup>6</sup>, Mukul Rameshchandra Jain<sup>3</sup>, Arun Kumar Trivedi<sup>2</sup>, Rakesh Maurya<sup>5</sup>, Madan Madhav Godbole<sup>7</sup>, Jiaur Rahaman Gayen<sup>8</sup>, Sabyasachi Sanyal<sup>2\*</sup> & Naibedya Chattopadhyay<sup>1\*</sup> (2015) Pathophysiological mechanism of bone loss in type 2 diabetes involves inverse regulation of osteoblast function by PPAR $\gamma$  coactivator-1 $\alpha$  and skeletal muscle atrogenes: adiponectin receptor 1 as a potential target for reversing diabetes-induced osteopenia. *Diabetes* 64, 2609-2623

66. Taran Khanam, Ankita Shukla, Niyati Rai & **Ravishankar Ramachandran** (2015) Identification of Critical Determinants for Substrate Recognition and Catalysis in the *M. tuberculosis* Class II AP-endonuclease/3'-5' Exonuclease III *Biochim. Biophys. Acta* 1854, 505-516, 2015

67. Aditi Chatterjee, Sapna Pandey, Pramod Singh, Navendu Pathak, Niyati Rai, **Ravishankar Ramachandran**, Ramapati Tripathi, & Kishore Srivastava (2015) Biochemical and functional characterizations of tyrosine phosphatases from pathogenic and non-pathogenic mycobacteria: Indication of phenyl cyclopropyl methyl-/ phenyl butenylazoles as tyrosine phosphatase inhibitors *Appl. Microbiol. Biotech.* 99, 7539-7548, 2015

68. Nisha Yadav<sup>1§</sup>, Taran Khanam<sup>2§</sup>, Ankita Shukla<sup>2</sup>, Niyati Rai<sup>2</sup>, Kanchan Hajela<sup>1#</sup> & **Ravishankar Ramachandran** (2015) Tricyclic dihydrobenzoxazepine and Tetracyclic indole derivatives can specifically target bacterial DNA ligases and can distinguish between the human DNA Ligase I *Organic & Biomolecular Chemistry*, **13**, 5475-5487, 2015

69. Taran Khanam, Niyati Rai & **Ravishankar Ramachandran** (2015) Mycobacterium tuberculosis class II apurinic/apyrimidinic-endonuclease/3'-5' exonuclease III exhibits DNA regulated modes of interaction with the sliding DNA  $\beta$ -clamp *Mol. Microbiol.* **98**, 46-68, 2015

70. Tripathi SM, Agarwal A & **Ravishankar Ramachandran** (2015) Mutational analysis of Mycobacterium tuberculosis lysine  $\epsilon$ -aminotransferase and inhibitor co-crystal structures, reveals distinct binding modes. *Biochem Biophys Res Commun* **463**, 154-160, 2015

71. Kapil Upadhyaya, Hamidullah, Kartikey Singh, Ashutosh Arun, Mahendra Shukla, Neetika Srivastav, Raghib Ashraf, Abhishek Sharma, Rohit Mahar, Sanjeev K. Shukla, Jayanta Sarkar, **Ravishankar Ramachandran**, Jawahar Lal, Rituraj Konwar and Rama Pati Tripathi (2016) Identification of Gallic acid based Glycoconjugates as a novel anti-tumor agents targeting tubulin polymerization *Organic & Biomolecular Chemistry* **14**, 1338-1358, 2016

72. Sonal Shree, Abhishek Kumar Singh, Richa Saxena, Harish Kumar, Aparna Agarwal, Vijay Kumar Sharma, Kanchan Srivastava, Kishore Kumar Srivastava, Sabyasachi Sanyal and **Ravishankar Ramachandran** (2016)

The *M. tuberculosis* HAD phosphatase (Rv3042c) interacts with host proteins and is inhibited by Clofazimine

*Cell. Mol. Life Sci.* **73**, 3401-3417

73. Abhishek Dey, Sonal Shree, Sarvesh Kumar Pandey, Rama Pati Tripathi & **Ravishankar Ramachandran** (2016)

Crystal Structure of *Mycobacterium tuberculosis* H37Rv AldR (rv2779c), a regulator of the ald gene: DNA-binding, and identification of small-molecule inhibitors

*J. Biol. Chem.* **291**, 11967-11980

74. Kumar A, Tripathi AK, Kathuria M, Shree S, Tripathi JK, Purshottam RK, **Ravishankar Ramachandran**, Mitra K, Ghosh JK. (2016)

Single amino acid substitutions at specific positions of the heptad repeat sequence of piscidin-1 yielded novel analogs that show low cytotoxicity as well as in vitro and in vivo anti-endotoxin activity

*Antimicrob. Agents Chemother.* **60**, 3687-3699.

75. Sapna Pandey, Aditi Chatterjee, Swati Jaiswal, Sanjay Kumar, **Ravishankar Ramachandran** & Kishore K Srivastava

Protein Kinase C- $\delta$  inhibitor, Rottlerin inhibits growth and survival of Mycobacteria exclusively through Shikimate Kinase

*Biochem Biophys Res Commun* **478**, 721-726, 2016

76. Abhishek K Singh; Sonal Shree; Sourav Chattopadhyay;

Sudhir Kumar; Anagha Gurjar; Sapana Kushwaha; Harish Kumar; Arun K

Trivedi; Naibedya Chattopadhyay; Rakesh Maurya; **Ravishankar Ramachandran**; Sabyasachi Sanyal (2017)

Small molecule adiponectin receptor agonist GTDF protects against skeletal muscle atrophy  
*Mol. Cell Endocrinol.* **439**, 273-285, 2017

77. Amit Kumar, Mahajan, Mukesh; Awasthi, Bhanupriya; Tandon, Anshika; Harioudh, Munesh; Shree, Sonal ; Singh, Pratiksha ; Shukla, Praveen K.; **Ravishankar Ramachandran**; Mitra, Kalyan; Bhattacharjya, Surajit; Jimut Ghosh (2017)

Piscidin-1-analogs with double L- and D-lysine residues at the interface of polar and non-polar faces exhibited different conformations in LPS but comparable *in vivo* anti-endotoxin activities  
*Sci. Rep.* **7**: 39925, 2017

78. Amit Gaur, Vijay K Sharma, Sonal Shree, Niyati Rai & **Ravishankar Ramachandran**

Characterization of EccA3, a CbbX family ATPase from the ESX-3 secretion pathway of *M. tuberculosis*

*Biochim. Biophys. Acta* **1865**, 715-724, 2017

79. Biochemical characterization and novel inhibitor identification of *Mycobacterium tuberculosis*

Endonuclease VIII 2 (Rv3297)

Kiran Lata, Mohammad Afsar & **Ravishankar Ramachandran** (2017)

*Biochem Biophys Rep* **12**, 20-28, 2017

80. Mycobacterial Protein tyrosine kinase A phosphorylates PtpA at Tyrosine residues and the mechanism is stalled by the novel series of inhibitors (2018)

Swati Jaiswal, Aditi Chatterjee, Sapna Pandey, Kiran Lata, Gadi Ranjith Kumar, Manda Rajesh, Sanjay Kumar, Maddi Sridhar Reddy, **Ravishankar Ramachandran** and Kishore K Srivastava

*Journal of Drug Targeting*, DOI: 10.1080/1061186X.2018.1473407, 2018

81. Leprosy drug clofazimine activates peroxisome proliferator-activated receptor- $\gamma$  and synergizes with imatinib to inhibit chronic myeloid leukemia cells.

Harish Kumar, Sourav Chattopadhyay, Nabanita Das, Sonal Shree, Dinesh Patel, Jogeswar Mohapatra, Anagha Gurjar, Sapana Kushwaha, Abhishek Kumar Singh<sup>1</sup>, Shikha Dubey<sup>3</sup>, Kiran Lata<sup>3</sup>, Rajesh Kushwaha<sup>5</sup>, Riyazuddin Mohammed, Krishnarup Ghosh Dastidar<sup>4</sup>, Namrata Yadav<sup>4</sup>, Achchhe Lal Vishwakarma<sup>7</sup>, Jiaur Rahaman Gayen<sup>6,2</sup>, Sanghamitra Bandyopadhyay<sup>5</sup>, Abhijit Chatterjee<sup>4</sup>, Mukul Rameshchandra Jain<sup>4</sup>, Anil Kumar Tripathi<sup>8</sup>, Arun Kumar Trivedi, Naibedya Chattopadhyay, **Ravishankar Ramachandran**, Sabyasachi Sanyal

*Haematologica*, **105**, 971-986, 2020

82. Structural-functional diversity of malaria parasite's PfHSP70-1 and PfHSP40 chaperone pair gives an edge over human orthologs in chaperone-assisted protein folding.

Mohammad Anas, Ankita Shukla, Aradhya Tripathi, Varsha Kumari, Chetan Prakash, Priyabrata Nag, L. Sathish, Sandeep K. Sharma, **Ravishankar Ramachandran** and Niti Kumar

*Biochem. J.*, **477**, 3625-3643, 2020

83. *M. tuberculosis* class II apurinic/aprimidinic-endonuclease/3'-5' exonuclease (XthA) engages with NAD<sup>+</sup>-dependent DNA ligase A (LigA) to counter futile cleavage and ligation cycles in Base Excision Repair

Taran Khanam, Mohammad Afsar, Ankita Shukla, Faiyaz Alam, Sanjay Kumar, Horam Soyar, Kunzes Dolma, Ashish, Mukesh Pasupuleti, Kishore Kumar Srivastava, Ravi Sankar Ampapathi & **Ravishankar Ramachandran\***

*Nucleic Acids Research*. **48**, 4325-4343, 2020

84. Structure based identification of first-in-class fragment inhibitors that target the NMN pocket of Mycobacterium tuberculosis NAD<sup>+</sup>-dependent DNA Ligase A

Ankita Shukla, Mohammad Afsar, Nelam Kumar, Sanjay Kumar & **Ravishankar Ramachandran\***

*J. Struct. Biol.*, **213**, 107655, 2021



85. [Fe-S] biogenesis and unusual assembly of the ISC scaffold complex in the Plasmodium falciparum mitochondrion.

Mohammad Sadik, Mohammad Afsar, **Ravishankar Ramachandran**, Habib S.

*Mol Microbiol.* **116**: 606-623, 2021

86. Salt bridges at the subdomain interfaces of the adenylation domain and active-site residues of Mycobacterium tuberculosis NAD<sup>+</sup>-dependent DNA ligase A (MtbLigA) are important for the initial steps of nick-sealing activity.

Afsar M, Shukla A, Kumar N & **Ravishankar Ramachandran\***

*Acta Crystallogr D Struct Biol.* **77**: 776-789, 2021

87. Mycobacterium tuberculosis Endonuclease VIII 2 (Nei2) forms a pre-replicative BER complex with DnaN: Identification, characterization, and disruption of complex formation.

Kiran Lata, Jyoti Vishwakarma, Sanjay Kumar, Taran Khanam, and **Ravishankar Ramachandran\***.

*Molecular Microbiology*, under revision, 2021