

CURRICULUM VITAE

Ajay Kumar Saxena
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Jawaharlal Nehru University
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New Delhi-110067, INDIA
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Education:

1990-1995 Ph.D. in Structural Biology, AIIMS, New Delhi, India.

Academic appointments:

03/2011- Professor, Structural Biology Section, Jawaharlal Nehru University, New Delhi, India
2005-2011 Associate Professor, Structural Biology Section, Jawaharlal Nehru University, New Delhi, India
1998-2005 Research Fellow, Structural Biology Section, LIG, NIAID, National Institutes of Health, Twinbrook, Maryland, USA
1996-1998 Postdoctoral Fellow, Institute of Biophysics & X-ray Structure Research, Austrian Academy of Sciences, Graz, Austria, Europe

Fellowships:

2012 Bill & Melinda gates foundation travel award for GRC
2005 NIH/NIAID special performance award
1998-2005 John E. Fogarty International Fellowship, National Institutes of Health, USA
1996-1998 Austrian Academy of Science Fellowship, Government of Austria, Austria
1995-1996 Senior Research Fellowship, Department of Biotechnology, India
1990-1994 Junior Research Fellowship, All India Institute of Medical Sciences, India
1988 National merit scholar

Extramural research funding

2018-2021 Department of Science and Technology (DST), India.
Title- Development of Single-cell derived clonal spheroids as a tool for drug discovery in **cancer research**. Co-PI- Ajay K. Saxena
2016-2019 Department of Science and Technology (DST), India.
Title- Structural and functional analysis of *M. tuberculosis* EccC+ EsxAB complex from ESX-1 virulence secretion system. PI-Ajay K. Saxena
2013-2016 University Potential of Excellence (JNU) India
Title: Structure and function analysis of *P. falciparum* **Pfs25 and Pfs28** proteins and their complexes with receptors. PI- Ajay K. Saxena
2013-2016 Department of Science and Technology (DST), India.
Title- Structure and function analysis of *M. tuberculosis* vaccine candidate **EspC** protein. PI-Ajay K. Saxena
2013-2016 Department of Biotechnology (DBT), India
Project- Structural and functional analysis of *M. tuberculosis* **DprE1 and DprE2** enzymes involved in cell wall synthesis. PI-Ajay K. Saxena & T. P. Singh

- 2011-2014 Council of Scientific and Industrial Research (CSIR), India.
Project-Structure analysis of *M. tuberculosis* CarD protein: an essential regulator of rRNA transcription. PI-Ajay K. Saxena
- 2010-2013 Department of Science and Technology (DST), India.
Project- Structural and functional analysis of ERG oncoprotein: potential target to develop prostate cancer drug. PI-Ajay K. Saxena
- 2006-2009 Council of Scientific and Industrial Research (CSIR), India.
Project- Structure analysis of the Human Transporter Associated with Antigen Processing (TAP) protein. PI-Ajay K. Saxena

Research interests:

- Structural and functional analysis of disease related proteins from *M. tuberculosis*, *Malaria* and *cancer*
- Structure guided drug/vaccine development

Editorial member/Journal reviewer:

- Reviewer:Nature communication, Nature Scientific Report, JBC, Biochemistry, Biochemical Journal, Molecular Biochemical Parasitology, BMC Biochemistry, PLoS One, BMC crystallography, Protein Science, IUCr journals
- Indian crystallographic association

Conference organized

- National seminar on Crystallography (NSC-42 in 2012 GIAN course-2017)
- Academic staff college refresher course-November 2018
- Summer school program-JNU-2019

TEACHING, THESIS SUPERVISION AND ADMINISTRATIVE EXPERIENCES

Teaching activity

- Molecular Biophysics course to Pre-Ph.D. students
- Membrane Biochemistry to M.S.-IV-year students
- Structural & Molecular Biology course to M.S. (III) year students
- Biophysics & Structural Biology course to M.S. (II) year students
- Physics for Biologist course to M.S. (I) year students
- Bioinformatics course to MS(III) year students

No. of Ph. D./M. tech/MS students supervised

- Ph. D.- 8 students
- M. Tech.- 15 students
- M.S.- 15 students

Administrative Positions/Activities

- Member-House allotment committee (2018-2020)
- Member of standing committee on recognized research institutes (2019-2021)
- Member-SCIC (July 26, 2018-2020)
- Member-SLS grievance committee (2019-2021)
- Member-Anti ragging committee, JNU (2019-2021)
- Concurrent faculty-School of Sanskrit (2019-2021)
- Member-Advisory committee AIRF (Nov 2017-2020)

- Member-purchase committee, SLS (2019-2021)
- Member-Budget and finance committee (2019)
- Member-School level grievance committee (2019)
- Member-Framing rule and disciplinary service in JNU (2018)
- Member-screening committee of selection of participant in HRDC (2018)
- Member- Purchase committee-SLS (2019)

Other Professional Activities

- Proctor, Jawaharlal Nehru University (2019-2021)
- Adjunct Professor, School of Sanskrit and Indic studies, JNU (2019-)
- Member, JNU-IMTECH Academic Committee (2019- 2021)
- Member, JNU-NII Academic Committee (2017- 2022)
- Member, JNU-CCMB Academic Committee (2018- 2020)
- Member, Academic Council JNU, (2020-2023)
- LEAP Program participant at JNU, New Delhi and NUS at Singapore (2019).

Conference organized

- National seminar on Crystallography (NSC-42 in 2012 GIAN course-2017)
- Academic staff college refresher course-November 2018
- Summer school program-JNU-2019

RESEARCH ACCOMPLISHMENTS

Project 1. Structure-function analysis of *M. tuberculosis* related proteins

In current program, we are working on *M. tuberculosis* key enzymes involved in cell wall biogenesis, ESX-1 secretion system and ESX-1 regulatory system. These projects are,

P1. Structural and functional characterization of (i) EccA1+EspC complex (ii) EccC+EsxAB complex and (iii) EspR/DNA regulator from *M. tuberculosis* ESX-1 secretion system

In current project, we have performed the structural and biochemical analysis of EccA1+EspC and EccC+EsxAB complexes and EspR regulator from *M. tuberculosis* ESX-1 secretion system. These studies have provided the avenues for structure based development of ant virulence inhibitors against mycobacteria.

P2. Structural and functional characterization of stress regulatory (i) Rv0081 protein (ii) MprA/MprB proteins (iii) CarD/RNAP complex proteins from *M. tuberculosis* ESX-1 secretion system

In current project, we have performed structural and biochemical analysis of various transcription factors involved in ESX-1 regulation, stress regulation and dormant stage of mycobacteria. These studies have provided avenue for drug development against dormant stage of mycobacteria.

P3. Structural and functional characterization of (i) GmhA/HddA/GmhB and (ii) DprE1/DprE2 (iii) PIMs enzymes involved in *M. tuberculosis* cell wall biogenesis

In current project, we have structurally and functionally characterized the (i) GmhA, HddA and GmhB enzymes involved in GDP-heptose biosynthetic pathway (ii) DrpE1/DprE2 enzymes involved in DPA biosynthetic pathway and looking forward for specific inhibitor/drug development against *M. tuberculosis*.

Project 2. Structure-function analysis of *Plasmodium* drug/vaccine candidate proteins

The malaria vaccine developers around the world are trying to develop all three types of malaria vaccines, pre-erythrocyte, blood stage and transmission blocking. In current program, we are working on following vaccine candidate proteins,

P1. Structural and functional characterization of *Plasmodium* P25/P28 proteins and their complexes with transmission blocking antibodies.

In current project, we have functionally and structurally characterized the *Plasmodium* P25 and P28 proteins and their complexes with Fab fragment of transmission blocking antibodies. These studies have provided clues about development of transmission blocking vaccines against Plasmodium.

P2. Structural and functional characterization of *Plasmodium* cysteine proteases (i) Falcipain/Falcipain and (iii) Metacaspases 2 &3.

In current project, we have structurally and functionally characterized the *Plasmodium* Falcipain-2, Falcipain-3, Metacaspase-2 and Metacaspase-3 enzymes, potential candidates for drug development against Plasmodium.

Project 3. Structure-function analysis of cancer related proteins

P1. Structural and functional characterization of human Ergp55 oncoprotein

In current project, we have structurally and functionally characterized the Ergp55 oncoprotein, a transcription factor of the ETS family. Ergp55 oncoprotein are the frequent targets for chromosomal translocation that results in various types of leukemia's and Erwing sarcoma.

P2. Structural and functional characterization of *C. albicans* Cdr1p multidrug transporter

The objective of this proposal was to analyze the structure and mechanism of Cdr1p, a major ABC transporter from *Candida albicans* using X-ray crystallography and Cryo-electron microscopic techniques. The multiple drug transporter Cdr1p is overexpressed in *Candida* cells and linked to clinical antifungal resistance. We have structurally and functionally characterized this transporter and looking forward drug development based on structures.

P3. Covid-19 related projects:

In current project, we worked on principle of multi-patch vaccine against Covid-19 and developed various antigenic epitopes critical for Covid-19 vaccination.

(1) Sukrit et. al., 2020, *J. Biomol. Struc. & Dynamics*, DOI: 10.1080 /07391102.2020.1838329 (2) Sukrit et. al., *JMIR Bioinformatics Biotechnol* 2020 1(1): e19371 (3) Sukrit et. al., 2019, *J. Biomol. Struc. & Dynamics*, 37(16): 4345–4360 (4) Sukrit et. al., 2018, *Infection and Drug Resistance* 11: 1–15.

PUBLICATIONS (# as corresponding author)

2021-2022

60. Yeshveer Singh, Ruby Sharma, Manasi Mishra, Praveen Kumar Verma and **Ajay K. Saxena# (2022)**. Crystal structure of ArOYE6 reveals a novel C-terminal fold and mechanistic insights into the distinct class III OYEs from pathogenic fungi. *The FEBS Journal*. 2022 Mar 21
59. Ruby Sharma, and **Ajay K. Saxena# (2022)**. Structural and functional analysis of cancer related proteins: A critical target for drug development.

58. S. Srivastava, S. Verma, M. Kamthania, D. Agarwal, **A. K. Saxena**, M. Kolbe, S. Singh, A. Kotnis, B. Rathi, S. A. Nayar, H. J. Shin, K. Vashith and K. C Pandey (2022). Computationally validated SARS-CoV-2 CTL and HTL Multi-Patch vaccines, designed by reverse epitomics approach, show potential to cover large ethnically distributed human population worldwide.
Journal of Biomolecular Structure and Dynamics, 40:5, 2369-2388.
57. Jawa Y, Yadav P, Gupta S, Mathan SV, Pandey J, **Saxena AK**, Kateriya S, Tiku AB, Mondal N, Bhattacharya J, Ahmad S, Chaturvedi R, Tyagi RK, Tandon V and Singh RP (2021) Current Insights and Advancements in Head and Neck Cancer: Emerging Biomarkers and Therapeutics with cues from single cell and 3D model omics profiling.
Front. Oncol. 11:676948.
56. Arkita Bandhopadhyay and **Ajay K. Saxena#** (2021). Structural and ATPase activity analysis of nucleotide binding domain of Rv3870 enzyme of *M. tuberculosis* ESX-1 system.
Int. J. Biol. Macromol 189: 879–889.
55. Vandana, R. Pandey, Srinivasan E., I. Kalia, A. P Singh, **Ajay K. Saxena**, R. Rajaekaran, D. Gupta, K. C. Pandey (2021). *P. falciparum* Metacaspases-2 captures its natural substrate in a noncanonical way.
The journal of Biochemistry 170 (5), 639-653
54. Sumita Karan, Ankita Behl, Amin Sagar, Arkita Bandhopadhyay and **Ajay K. Saxena#** (2021). Structural studies on *Mycobacterium tuberculosis* HddA enzyme using small angle X-ray scattering and dynamics simulation techniques,
Int. J. Biol. Macromol. 171:28-36.
53. Sukrit Srivastava, **Ajay K. Saxena**, Michael Kolbe (2021). Exploring the structural basis to develop efficient multi-epitope vaccines displaying interaction with HLA and TAP and TLR3 molecules to prevent NIPAH infection, a global threat to human health.
BioRxiv doi: <https://doi.org/10.1101/2021.09.17.460735>
52. R Sharma, VK Kashyap, M. Kumar, A Bansal, **Ajay K. Saxena#** (2021). Dissection of function and recognition mechanism of *M. tuberculosis* ESX-1 secreted virulence factor EspC
BioRxiv <https://doi.org/10.1101/2021.09.24.461649>
51. Arkita Bandhopadhyay and **Ajay K. Saxena#** (2021). Structural and biochemical analysis of ATPase activity and EsxAB substrate binding of *M. tuberculosis* EccCb1 enzyme.
BioRxiv preprint doi: <https://doi.org/10.1101/2021.05.31.446396>.
- 2016-2020**
50. S. Karan, B. Pratap, Shiv P. Yadav, FNU. Ashish & **Ajay K. Saxena#** (2020). Structural and functional characterization of *M. tuberculosis* sedoheptulose-7-phosphate isomerase, a critical enzyme involved in lipopolysaccharide biosynthetic pathway.
Nature Sci. Rep. 10(1), 1-16.
49. S. P. Gangwar, A. Bandyopadhyay and **Ajay K. Saxena#** (2020). Structural studies on *M. tuberculosis* decaprenyl phosphoryl- β -Dribose epimerase-2 enzyme involved in cell wall biogenesis.

48. Srivastava S, Verma S, Kamthania M, Kaur R, Badyal RK, **Saxena AK**, Shin HJ, Kolbe M, Pandey KC (2020). Structural Basis for Designing Multi-epitope Vaccines Against COVID-19 Infection: In Silico Vaccine Design and Validation. *JMIR Bioinform Biotech. 1(1): e19371.*
47. S. Srivastava, M. Kamthania, R. K. Pandey, **A. K. Saxena**, V. Saxena, S. K. Singh, R. K. Sharma & N. Sharma (2019). Design of novel multi-epitope vaccines against severe acute respiratory syndrome validated through multistage molecular interaction and dynamics *Journal of Biomolecular Structure and Dynamics, 37:16, 4345-4360*
46. Bhumika Kumar, Deepak Singla, Mohammad Kashif, Ruby Sharma, Rajnikant Dixit, Agam P. Singh, **Ajay K. Saxena**, Mohammad Abid, Kailash C. Pandey (2019). Metacaspase-3 of *Plasmodium falciparum*: An atypical trypsin-like serine protease. *Int. J. Biol. Macromol. 138: 309-320.*
45. Sumita Karan, Bhanu pratap, Ashish, **Ajay K. Saxena#** (2019). Low-resolution SAXS and structural dynamics analysis on *M. tuberculosis* GmhB enzyme involved in GDP-heptose biosynthetic pathway. *Int. J. Biol. Macromol. 136: 676-685.*
44. R. Pasupureddy, S. Verma, A. Pant, R. Sharma, **A. K. Saxena**, R. Dixit, S. Seshadri, K. C. Pandey (2019). Crucial residues in falcipains that mediates hemoglobin hydrolysis. *Experimental Parasitology 197:43-50.*
43. A. Pant, R. Kumar, N. Ahmed Wani, S. Verma, R. Sharma, S. Sharma, V. Pande, **A. K. Saxena**, R. Dixit, R.K. Rai and K. C. Pandey (2018). Allosteric Site Inhibitor Disrupting Auto-processing of Malarial Cysteine Proteases *Nature Sci. Rep. 8(1): 1-15.*
42. Srivastava S, Kamthania M, Singh S, **Saxena AK**, Sharma N. (2018). Structural basis of development of multi-epitope vaccine against Middle East respiratory syndrome using in silico approach. *Infect Drug Resist. 11:2377-2391.*
41. R. Sharma, S. P. Gangwar, **A. K. Saxena#** (2018). Comparative structure analysis of ETSi domain of ERG3 and its complex with E74 promoter DNA sequence *Acta Crystallogr. Section F Biol. Crystallogr. section 74(10): 656-663.*
40. K. Ahuja, M. A. Beg, R. Sharma, **A. K. Saxena**, N. Naqvi, N. Puri, A. Chaudhury, R. Duncan, P. Salotra, H. Nakhasi, A. Selvapandiyani (2018). Importance of threshold expression of a novel trypanosome specific glycosomal protein for the growth of *Leishmania donovani* parasites. *BBA-Molecular Cell Research 1865(8):1148-1159.*
39. Agam P Singh, Jitendra Singh, Ruby Sharma, Mymoona Akhter, Pradyumna K Mishra, **Ajay K. Saxena**, Rajnikant Dixit, Brijesh Rathi, Anju Katyal, Kailash C Pandey (2018). Biochemical characterization of unusual cysteine protease of *P. falciparum*, metacaspase-2 (MCA-2) *Molecular & Biochemical Parasitology 220: 28-41.*

38. S. Karan, V. K. Kashyap, S. Shafi and **A. K. Saxena#** (2017). Structural and inhibition analysis of novel sulfur rich 2-mercapto benzothiazole and 1,2,3- triazole ligands against *Mycobacterium tuberculosis* DprE1 enzyme.
J. Mol. Model. 23(8):1-11.
37. M. K. Rawal, A. Banerjee, A. H. Shah, M. F. Khan, S. Sen, **A. K. Saxena**, B. C. Monk, R. D. Cannon, R. Bhatnagar, A. K. Mondal & R. Prasad (2016). Newly identified motifs in *Candida albicans* **Cdr1** protein nucleotide binding domains are pleiotropic drug resistance subfamily-specific and functionally asymmetric.
Nature Sci. Rep. 6:27132.
36. S. R. Meena and **A. K. Saxena#** (2016). Structure of *E. coli* GroEL in substrates and ADP unloaded state (PDB-4HEL)
J. Phys. Chem. Biophys. 6 (222), 2161-0398.10002

2011-2015

35. A. H. Shah, M. K. Rawal, **A. K. Saxena**, Mondal, A. and R. Prasad (2015). ABC transporter **Cdr1p** harbors a critical acid/base pair of between intracellular loop and nucleotide-binding domain important for protein trafficking.
FEMS Yeast Res. 15(5). pii: fov036.
34. A. H. Shah, M. K. Rawal, S. Dhamgaye, S. S. Komath, **A. K. Saxena** and R Prasad (2015). Mutational Insight into Intracellular loops defines cross talk between NBDs and ICLs of the yeast ABC transporter **Cdr1p**.
Nature Sci. Rep. 5(1): 1-17.
33. S. Sundararaj, **A. K. Saxena**, R. Sharma, K. Vashisht, S. Sharma, A. Anvikar, R. Dixit, K. C. Pandey (2014). Hydrophobic interaction and hydrogen bond within the BC loop are interacting within the active site of *cysteine proteases* of *P. falciparum* and *P. vivax*
PLoS ONE, 9(4): e93008.
32. S. P. Gangwar, S. R. Meena and **A. K. Saxena#** (2014). Comparison of different crystal forms of ESX-1 secreted protein regulator *EspR* from *M. tuberculosis* and its implication for protein regulator activity (PDB-4NDW)
Acta Crystallogr. Section F Biol. Crystallogr. Section F 70(4), 433-437.
31. S. P. Gangwar, S. R. Meena and **A. K. Saxena#** (2014). Crystal structure of carboxy-terminal domain of *M. tuberculosis* *CarD* protein: an essential rRNA transcriptional regulator (PDB-4KMC).
Acta Crystallogr. Section F Biol. Crystallogr. Section F 70(2), 160-165.
30. M. K. Rawal, M. F. Khan, K. Kapoor, N. Goyal, S. Sen, **A. K. Saxena**, A. M. Lynn, Joel D. A., Tyndall, B. C., Monk, R. D. Cannon and R. Prasad (2013). Insight into PDR ABC pump drug transport through mutagenesis of **Cdr1p** transmembrane domains
J. Biol. Chem. 288(34), 24480-24493
29. Gangwar, S. P., Dey, S. and **Saxena, A. K.#** (2012). Structural modeling and DNA binding auto-inhibition analysis of **Ergp55**, a critical transcription factor in prostate cancer.
PLoS ONE 7(6): e39850.

28. S. Sundararaj, D. Singh, **A. K. Saxena**, P. S. Sijwali, R. Dixit, K. C. Pandey (2012). The ionic and hydrophobic interactions are required for the activation of cysteine proteases of *P. falciparum*. *PLoS ONE* 7(10): e47227.
27. **A. K. Saxena#** (2012). Structure of Fab fragment of malaria transmission- blocking antibody 2A8 against *P. vivax* P25 protein. (PDB-3S62) *Int. J. Biol. Macromol.* 50, 153-156.
26. Sita R. Meena, S. P. Gangwar and **A. K. Saxena#** (2012). Purification, crystallization and preliminary X-ray crystallographic analysis of ATPase domain of TAP in nucleotide free, ADP, vanadate and azide inhibited form. *Acta Crystallogr. Section F Biol. Crystallogr.* 68(6), 655-658.
25. S. P. Gangwar, Sita R. Meena and **A. K. Saxena#** (2012). Purification, crystallization and preliminary X-ray crystallographic analysis ETS domain of Ergp55 in complex with cfo promoter DNA sequence. *Acta Crystallogr. Section F Biol. Crystallogr.* 68(11), 1333-1336.
24. **A. K. Saxena#** (2012). Structural and functional analysis of key proteins involved in ESX-1 secretion system of *M. tuberculosis*: novel targets for drug developments *J. Anal. Bioanal. Techniques* 3, 7 (Conference paper)
23. S. P. Gangwar, S. R. Meena and **A. K. Saxena#** (2011). Cloning, purification, crystallization and preliminary X-ray analysis of EspR: a secreted transcription factor from *M. tuberculosis*. *Acta Crystallogr. Section F Biol. Crystallogr.* 67(1), 83-86.
22. **A. K. Saxena#** and S. P. Gangwar (2011). Structural and functional dissection of Ergp55 oncoprotein. *J. Anal. Bioanal. Techniques* 2, 6 (Conference paper)

2006-2010

21. A. Manford, T. Xia, **A. K. Saxena**, C. Stefan, F. Hu, S. D. Emr and Y. Mao (2010). Crystal structure of the yeast Sac1: implications for its phosphoinositide phosphatase function (PDB-3LWT). *EMBO J.* 29(9), 1489-1498.
20. Sharma, B., Ambedkar R. D. and **Saxena, A. K.#** (2009). A very large C-loop in EGF domain IV is characteristic of the *Plasmodium* P28 family of ookinete surface proteins. *J. Mol. Model* 15(3), 309-321.
19. Sharma B., Jaiswal M. K. and **Saxena, A. K.#** (2009). EGF domain II of protein Pb28 from *P. berghei* interacts with monoclonal transmission blocking anti- body 13.1. *J. Mol. Model* 15(4), 369-382.
18. **Saxena, A. K.#**, Yimin, W. and Garboczi, D. N. (2007). *Plasmodium* P25 and P28 surface proteins: Potential malaria transmission blocking vaccines. *Eukaryotic Cell* 6(8), 1260-1265.

17. **Saxena, A. K.**, Singh, K., Su, H.P., Klein, M. M., Stower, A. W., Saul, A. J., Long, C. and Garboczi, D. N. (2006). *Plasmodium* P25 and P28, essential proteins for survival of the malaria parasite in the mosquito are tile-like triangular prism (**PDB-1Z27, 1Z1Y, 1Z3G**). *Nature (Struc. & Mol. Biol.)* 13(1), 90-91.
16. C. Chen, **A. K. Saxena**, W. N. Simcoke, D. N. Garboczi, P. L Pedersen and Y.H. Ko (2006). MITOCHONDRIAL ATP SYNTHASE: crystal structure of the catalytic F1 unit in a Vanadate-induced transition-like state and implications for mechanism (**PDB-2F43**). *J. Biol. Chem.* 281(19), 13777-13783.

2001-2005

15. **Saxena, A. K.**, Singh, K., Long, C. and Garboczi, D. N. (2004). Preparation, crystallization and preliminary x-ray analysis of complex between antibody and *P. vivax* sexual stage 25kDa protein Pvs25 and malaria transmission- blocking antibody Fab fragment. *Acta Crystallogr. D Biol. Crystallogr.* 60(11), 2054-2057.
14. **Saxena, A. K.**, Saul, A. and Garboczi, D. N. (2004). Crystallization and preliminary X-ray analysis of the *P. vivax* sexual stage 25kD protein, Pvs25, a transmission-blocking vaccine candidate for malaria. *Acta Crystallogr. D Biol. Crystallogr.* 60(4), 706-708.

1996-2000

13. **Ajay K. Saxena**, C. Betzel and T. P. Singh (2000). Structure of a Ternary Complex of Proteinase K, Mercury and A Substrate Analogue Heptapeptide Amide Ac-Pro-Ala-Pro-Phe-Ala-Ala-Ala NH₂, at 2.3 Å Resolution *Indian Journal of Physics* 74, 187-194
12. **Saxena, A. K.**, Gries A, Schwarzenbacher, R., Kostner, G. M., Laggner, P. and Prassl, R. (1998). Crystallization and preliminary X-ray crystallographic studies on Apolipoprotein-H from human plasma. *Acta Crystallogr. D Biol. Crystallogr.* 54(6), 1450-1452.
11. P Laggner, R Prassl, A Saxena, F Nigon, M Sara, S Eschenburg, C Betzel, JM Chapman (1997). Crystallization and preliminary x-ray crystallography of a low density lipoprotein from human plasma. *BIOPHYSICAL JOURNAL* 72 (2), THAM3-THAM3
10. Prassl, R., Chapman, J M., Nigon, F., Sara, M., Eschenburg, S., Betzel, C., **Saxena, A. K.** and Laggner, P. (1996). Crystallization and preliminary X-ray analysis of Low-Density Lipoprotein (**LDL**) from human plasma. *J. Biol. Chem.* 271(46), 28731-28733.
9. **Saxena, A. K.**, Singh, T. P., Peters, K., Fittkau, S., Visanji, M., Wilson, K. S. and Betzel, C. (1996). Structure of a ternary complex of Proteinase K, Hg and a substrate analogue hexapeptide N-Ac-Pro-Ala-Pro-Phe-Pro-Ala-NH₂ at 2.2-Å resolution (**PDB-1PJ8**). *Proteins, Struc. Funct. & Genet.* 25 (2), 195-201.
8. **Saxena, A. K.**, Singh, T. P., Peters, K., Peters, K., Fittkau, S. and Betzel, C. (1996). Strategy to design peptide inhibitors: Structure of the complex of Proteinase K with designed

octapeptide inhibitor N-Ac-Pro-Ala-Pro-Phe-DAla- (Ala)₃-NH₂ at 2.5 Å resolution (**PDB-1PFG**).

Protein Science 5(12), 2453-2458.

7. Singh, T. P. Padmanabhan, B. Narula, P. **Saxena, A. K.**, Betzel, C., Sharma, P. and Dey, S. (1996). Design of a specific peptide structure and subtilisin inhibitor using dehydro residues. *Adv. Exp. Med. Biol.* 379, 11-20.

1990-1995

6. **Saxena, A. K.**, Sharma, P. and Singh, T. P. (1995). Solid-state conformation of model dehydro-Phe containing peptide N-Ac-dehydro-Phe-L-Val-OH/OCH₃ in various solvents. *Ind. J. Phys.* 69A(3), 307-321.
5. Khanna, A., Khandelwal, B. L., **Saxena, A. K.**, and Singh, T. P. (1995). Di-chloro methane assisted oxidation of Pt (O) via cleavage of Te-Carbonyl bond of an asymmetric Telluride leading to the formation of Trans-[PtCl(Ar)(PPh₃)₂]. *Polyhedron* 14(19), 2705-2710.
4. Singh, A. K., Srivastava, V., Basumatary, J. K., Singh, T. P. and **Saxena, A. K.** (1994). Triphenyl Tellurium (IV) diethyldithiocarbamate: Synthesis and crystal structure of new example showing sterically sensitive long Te-S bonds. *Phosphorous Sulfur and Silicon* 89(1-4), 31-37.
3. **Saxena, A. K.**, Singh, T. P., Betzel, Ch., Visanji, M., Peters, K. and Fittkau, S. (1993). Structure of a ternary complex of Proteinase K, Hg²⁺ and substrate analogue hexapeptide N-Ac-Pro-Ala-Pro-Phe-Pro-Ala-NH₂. *Acta Crystallogr. A49 (Supplement), C106*.
2. Srivastava, V., Basumatary, J. K., Singh, A. K., Singh, T. P. and **Saxena, A. K.** (1993). Synthesis and crystal structure of Triphenyl Tellurium (IV) Ethylxanthate: An example of enhancement of the coordination number of Tellurium through long Te-S bonds. *Phosphorous Sulfur and Silicon* 85 (1-4), 175-181.
1. **Saxena, A. K.**, Sinha, S. K. and Singh, T. P. (1991). Structure of a carcinogenic Agent: 1-Formyl-3-Thiosemicarbazide. *Acta Crystallogr. Section C* 47(11), 2374-2376.

INVITED TALKS

- 2022 **Ajay K. Saxena (2022)**. Structural basis of development of anticancer drug against human Ergp55 oncoprotein. *Recent Trends in Cancer Prevention and Interception – Bench to Bedside*, School of Life Sciences and Special Centre for Systems Medicine, Jawaharlal Nehru University (JNU), New Delhi, India on 22-23 February 2022 (Chair)
- 2021 Sumita Karan, Ramesh Kumar and **Ajay K. Saxena (2021)**. Structure and mechanism of key enzymes involved in GDP-Heptose biosynthetic pathway in *M. tuberculosis*: potential drug target. *48th National Seminar on Crystallography November 25-27, 2021 Indian Institute of Technology Roorkee*, India.

- 2019 **Ajay K. Saxena (2019)**. Invited talk on Structure and biochemical analysis of *Plasmodium* cysteine proteases and its complexes with inhibitors/substrates, National, *Indian Society for Parasitology (ISP) and Special Centre for Molecular Medicine (JNU) Global impact of parasitic pathogens*, September 26, JNU, New Delhi.
- 2019 Ajay K. Saxena (2019) Invited talk on Structure and biochemical analysis of Plasmodium cysteine proteases and its complexes with inhibitors/substrates, National, *Indian Society for Parasitology (ISP) and Special Centre for Molecular Medicine (JNU) Global impact of parasitic pathogens*, September 26, JNU, New Delhi.
- 2018 Ruby Sharma, Kailash C. Pandey and **Ajay K. Saxena (2018)**. Crystal structure and biochemical analysis of *P. falciparum* cysteine protease Inhibitor Falstatin and its complex with cysteine protease (s). *46th National Seminar on Crystallography (NSC), June 2018* at NIMHANS, Bengaluru.
- 2015 Shanti P. Gangwar, Ruby Sharma and **Ajay K. Saxena (2015)**. Structural and functional Analysis of human Ergp55 oncoprotein. International Symposium on “*Current Advances in Radiobiology, Stem Cells and Cancer Research*” organised by *Cancer Research and Care Academy (CRCA)*, February 19-21, 2015, School of Life Sciences, Jawaharlal Nehru University, New Delhi.
- 2015 Ruby Sharma, Shanti P. Gangwar and **Ajay K. Saxena (2015)**. Structural and functional Analysis of human Ergp55 oncoprotein. Poster Presenta- tion (EMP139) *at 56th Association of Microbiologists of India (AMI)* 8-10th December, 2015, Jawaharlal Nehru University, New Delhi.
- 2012 **Ajay K. Saxena et. al.**, New insights in understanding the structure and mechanism of *Plasmodium* P25 and P28 proteins. *Gordon research conference* on host-parasite interaction, biology of, June 10-15, Salver Regina University, Providence, RI, USA.
- 2012 **Ajay K. Saxena et. al.**, New insights in understanding the structure and mechanism of *Plasmodium* P25 and P28 proteins. *Gordon research conference* on host-parasite interaction, biology of, June 10-15, Salver Regina University, Providence, RI, USA.
- 2010 Shanti P. Gangwar, Sita R. Meena and **Ajay K. Saxena**. Structural and functional analysis of EspR: a secreted transcription factor that control *M. tuberculosis* virulence. *Gordon research Conference* on Diffraction methods in Structural Biology, July 18-23, Lewiston, ME, USA.
- 2010 **Ajay K. Saxena**, Shanti P. Gangwar and Sita R. Meena. Structure analysis of ERG oncoprotein: a potential target to develop prostate cancer drug. *Gordon research Conference* on protein folding dynamics, January 9-10, Ventura, CA, USA.

CONFERENCE PAPERS

2022. Ruby Sharma, Vaishali Saxena and Ajay K. Saxena (2022). Structural and functional analysis of Ergp55 oncoprotein and protein kinases involved in cancer. *Recent Trends in Cancer Prevention and Interception – Bench to Bedside*. School of Life Sciences and Special Centre for Systems Medicine, Jawaharlal Nehru University (JNU), New Delhi, India on 22-23 February 2022 (Chair)

- 2021 **Saxena A. K. (2021)** Workshop on “Strategy for future EMBL research in the Life Sciences in Hamburg”, March 29, Hamburg, Germany.
- 2021 Arkita Bandyopadhyay and **Ajay K. Saxena (2021)**. Structural and functional characterization of ATPase domain of Rv3870 of *M. tuberculosis* ESX-1 system. 78th Pittsburgh Diffraction Conference (Virtual), 19th -21st September, SLAC, Stanford. (Poster presentation)
- 2021 Arkita Bandyopadhyay and **Ajay K. Saxena (2021)**. Structural and functional characterization of ATPase domain of Rv3870 of *M. tuberculosis* ESX-1 system. EMBO Virtual workshop on Designing functional biomolecular assemblies: Beyond biology, 28th September – 1st October, Heidelberg. (Poster presentation)
- 2021 Arkita Bandyopadhyay and **Ajay K. Saxena (2021)**. Structural and functional characterization of Rv3871 of *M. tuberculosis* ESX-1 system. EMBL Conference: Bringing Molecular Structure to Life: 50 Years of the PDB (Virtual), 20th - 22nd October, Heidelberg.
- 2021 Arkita Bandyopadhyay and **Ajay K. Saxena (2021)**. Structural and functional characterization of ATPase domain of Rv3870 of *M. tuberculosis* ESX-1 system. International Symposium on "Cellular Structural Biology & Bioimaging" (Virtual), 26th–27th October, Paul Scherrer Institute, Switzerland.
- 2021 Arkita Bandyopadhyay and **Ajay K. Saxena (2021)**. Structural and functional characterization of ATPase domain of Rv3870 of *M. tuberculosis* ESX-1 system. Protein Structure Determination in Industry 2021 Virtual Meeting (PSDI) (Virtual), 8th -10th November, PDBe.
- 2021 Arkita Bandyopadhyay, Ramesh Kumar, Swati Srivastava and **Ajay K. Saxena (2021)**. Structural and functional analysis of key enzymes involved in *M. tuberculosis* ESX-1 secretion system: novel targets for drug developments. 48th National Seminar on Crystallography (NSC-48), 25th -27th November, Department of Biosciences and Bioengineering, Indian Institute of Technology, Roorkee, India. **(Best Poster presentation)**
- 2021 Arkita Bandyopadhyay and **Ajay K. Saxena (2021)**. Structural and ATPase activity analysis of nucleotide binding domain of Rv3870 enzyme of *M. tuberculosis* ESX-1 system. 3rd National Biomedical Research Competition, Society of Young Biomedical Scientists, India, 6th – 10th December. **(Best Poster presentation)**
- 2021 Arkita Bandyopadhyay and **Ajay K. Saxena (2021)**. Structural and functional characterization of EccCb1 of *M. tuberculosis* ESX-1 system. 90th Annual Meeting of SBC(I) "Metabolism to Drug Discovery: Where Chemistry and Biology Unite" (Virtual), 16th -19th December, Amity Institute of Biotechnology & Amity Institute of Integrative Sciences and Health, Amity University Haryana (AUH), Gurugram, India. **(Best Poster presentation)**
- 2021 Saxena A. K. **(2021)** Workshop on “Strategy for future EMBL research in the Life Sciences in Hamburg”, March 29, Hamburg, Germany
- 2020 Arkita Bandyopadyay and **Ajay K. Saxena (2020)**. India-EMBO symposium on Microbial heterogeneity and Host tissue Tropism. 11-15 February, New Delhi.

- 2019 Ajay K. Saxena (2019) Invited talk on Structure and biochemical analysis of *Plasmodium* cysteine proteases and its complexes with inhibitors/substrates, National, Indian Society for Parasitology (ISP) and Special Centre for Molecular Medicine (JNU) Global impact of parasitic pathogens, September 26, JNU, New Delhi.
- 2019 Sumita Karan and Ajay K. Saxena (2019) Structure function analysis of enzymes involved in GDP-heptose biosynthetic pathway, Biospark, JNU, New Delhi.
- 2018 Ruby Sharma, Kailash C. Pandey and **Ajay K. Saxena (2018)**. Crystal structure and biochemical analysis of *P. falciparum* cysteine protease Inhibitor Falstatin and its complex with cysteine protease (s). 46th National Seminar on Crystallography (NSC), June 2018 at NIMHANS, Bengaluru.
- 2018 Ruby Sharma, Kailash C. Pandey and **Ajay K. Saxena (2018)**. Crystal structure and biochemical analysis of *P. falciparum* cysteine proteases and its complexes with inhibitors/substrates. Science Day Celebrations at Jawaharlal Nehru University, New Delhi, 28 Feb, 2018.
- 2018 Ruby Sharma, Srinivasan Sundararaj, Kailash C. Pandey, **Ajay K. Saxena (2018)**. Crystal structure and biochemical analysis of *Plasmodium falciparum* falstatin in complex with *Plasmodium* cysteine proteases FP2 and FP3. Poster presentation at Science Day Celebrations at Jawaharlal Nehru University, 28 Feb, New Delhi.
- 2017 Ruby Sharma, Srinivasan Sundararaj, Kailash C. Pandey, **Ajay K. Saxena (2017)**. Structural and Biochemical analysis of *P. falciparum* Falstatin in complex with *P. falciparum* cysteine proteases Falcipain-2 and Falcipain. 3rd Poster Presentation (EBS - 19) 86th Conference of Society of Biological Chemists' SBC Emerging Discoveries in Health and Agricultural Sciences' School of Life Sciences, Jawaharlal Nehru University, 16-19 November, New Delhi.
- 2016 S. Gaurinath and **Ajay K. Saxena, (2016)**. Conducted MHRD scheme Global Initiative for Academic Network (GIAN). Latest Methods in X-ray Crystallography: Lecture Series and Practical Course at JNU. Nov 14-25, School of Life Sciences, Jawaharlal Nehru University, New Delhi-110067, INDIA.
- 2016 **Ajay K. Saxena et. al. (2016)**. Structural and functional analysis of key proteins involved in ESX-1 protein secretion system of *M. tuberculosis*: novel targets for drug developments. Science Day, February 26, Jawaharlal Nehru University, New Delhi, India.
- 2015 Ruby Sharma, Shanti P. Gangwar and **Ajay K. Saxena**. Structural and functional Analysis of human Ergp55 oncoprotein. Poster Presentation at International Symposium on Current Advances in Radiobiology, Stem Cells and Cancer Research, February 19-21, 2015, School of Life Sciences, Jawaharlal Nehru University, New Delhi.
- 2015 Shanti P. Gangwar, Ruby Sharma and **Ajay K. Saxena**. Structural and functional Analysis of human Ergp55 oncoprotein. 56th International Conference "Association of Microbiologists of India (AMI) 2015" 07 -10 December, 2015 at JNU Convention Centre, New Delhi, India.

- 2014 Ruby Sharma, Srinivasan Sundararaj, Kailash C. Pandey and **Ajay K. Saxena (2014)** Mechanism of Interaction of Falstatin, Plasmodium Cysteine Protease Inhibitor with Cysteine Protease(s). Poster Presentation at Indo US Conference and Workshop on *Recent Advances on Structural Biology & Drug Discovery* on Oct 9-11, 2014 at Department of Biotechnology, IIT Roorkee, India.
- 2013 **Ajay K. Saxena et. al.**, Structure and function analysis of human Ergp55 oncoprotein, a critical transcription factor involved in prostate cancer *American Society of Cell Biology Annual Meeting*” held on December 14-18, 2013, New Orleans, LA, USA.
- 2012 **Ajay K. Saxena et. al.**, New insights in understanding the structure and mechanism of *Plasmodium* P25 and P28 proteins. *Gordon research conference* on host-parasite interaction, biology of, June 10-15, Salver Regina University, Providence, RI, USA.
- 2012 Shanti P. Gangwar, Sharmistha Dey and **Ajay K. Saxena**. Structural and functional dissection of Ergp55 protein. *National symposium of microbes in Health and Agriculture*, March 12-13, JNU, New Delhi, India.
- 2012 Shanti P. Gangwar, Sita R. Meena and **Ajay K. Saxena**. Structure and functional analysis of key proteins involved in *Mtb* ESX-1 protein export pathway: potential drug targets. *National symposium of microbes in Health and Agriculture*, March 12-13, JNU, New Delhi, **India**. (Best poster presentation award)
- 2011 Shanti P. Gangwar, Sita R. Meena and **Ajay K. Saxena**. Structural and functional analysis of secreted transcription factor EspR of *M. tuberculosis*. *Indo-NIAID Forum on TB drug discovery research*, April 20-21, New Delhi, India.
- 2010 Sita R. Meena, Shanti P. Gangwar and **Ajay K. Saxena**. Elucidation the mechanism of ATP hydrolysis cycle of the Transporter Associated with Antigen Processing (TAP). *4th International symposium on recent trends in macromolecular structure and function*, January 21-23, Chennai, India. (Best poster presentation award)
- 2009 **Ajay K. Saxena**, Shanti P. Gangwar and Sita R. Meena. Structure analysis of ERG Oncoprotein: a potential target to develop prostate cancer drugs. *International Conference on Protein Misfolding and Misprocessing in Disease*, NIH, USA.
- 2008 Sita R. Meena, Shanti P. Gangwar and **Ajay K. Saxena**. Structure analysis of Transporter Associated with Antigen Processing (TAP). *International Symposium on Novel Strategies for Targeted Prevention and Treatment of Cancer*, JNU, India.
- 2008 Shanti P. Gangwar, Sita R. Meena and **Ajay K. Saxena**. Structure analysis of ERG oncoprotein: a potential target to develop prostate cancer drug. *International Symposium on Novel Strategies for Targeted Prevention and Treatment of Cancer*, JNU, India.
- 2007 Sita R. Meena and **Ajay K. Saxena**. Structure analysis of Transporter As- sociated with Antigen Processing (TAP). *Satellite Symposium on Advancing Nanotechnology and Its Implications in Biological Sciences*, JNU, India.
- 2007 **Saxena, A. K.**, Sharma, B. and Amabedkar, R. Structure of P25 proteins from *Plasmodia* and their interactions with transmission-blocking antibodies: a molecular modeling and docking study. *One Hundred Years of Tropical Medicine*, London, UK.

- 2003 31st Annual Mid-Atlantic Protein Crystallography Workshop, Durham, North Carolina, USA, June 22-23, 2003.
- 2002 30th Annual Mid-Atlantic Protein Crystallography Workshop, NCI-Frederick, Maryland, USA, May 3-4, 2002.
- 2001 29th Annual Mid-Atlantic Protein Crystallography Workshop, College of William and Mary, Williamsburg, Virginia, USA, May 23-25, 2001.
- 1999 Workshop on ABC Transporters and Human Diseases, Division of Basic Sciences, National Cancer Institute, National Institutes of Health, Bethesda, Maryland, USA, Sept. 12-14, 1999.
- 1999 Workshop on Membrane Proteins, 7th Floor, Clark Hall, Cornell University, Ithaca, New York, USA, June 22-23, 1999.
- 1999 Mid-Atlantic Workshop, Centre for Advanced Research in Biotechnology (CARB), Maryland, USA, April 28-30, 1999.
- 1999 Second AAPS frontier symposium: Membrane Transporter and Drug Therapy, National Institute of Health, Bethesda, Maryland, USA, 8-10 April, 1999.
- 1999 Gordon Research Conference: Ligand Recognition and Molecular Gating, Ventura, California, USA, 7-12 March 1999.
- 1998 American Crystallographic Association (ACA) Annual Meeting, Arlington, Virginia, USA, 18-23 July, 1998.
- 1998 Mid-Atlantic Workshop John Hopkins University, Baltimore, Maryland, USA, 11-13 June, 1998.
- 1997 **Saxena, A. K.**, Prassl, R., Chapman, J. M., Sara, M. and Laggner, P.; Crystallization and Preliminary X-ray Analysis of Human Plasma Low Density Lipoprotein. Seventeenth European Crystallographic Meeting (ECM-17) I. S. T. Lisbon- Portugal, 24- 28 August 1997.
- 1997 **Saxena, A. K.**, Prassl, R., Chapman, J. M., Sara, M. and Laggner, P. ; Crystallization and Preliminary X-ray Analysis of Human Plasma Low Density Lipoprotein. American Crystallographic Association (ACA) Annual Meeting, St. Louis, Missouri, USA, 19-25 July 1997.
- 1995 **Saxena, A. K.**, Betzel, Ch. and Singh, T. P.; Structures of the complexes of Proteinase K and designed Oligopeptides. International Seminar-Cum School on Macromolecular Crystallographic Data, Saha Institute of Nuclear Physics, Calcutta, 16-20 November 1995.
- 1995 **Ajay K. Saxena**, Tej. P. Singh, Klaus Peters, Siegfried Fittkau, Marcia Visanji and Ch. Betzel ; Structure of a complex of proteinase K with a substrate analogue Octapeptide Inhibitor Ac -Pro-Ala-Pro-Phe-D-Ala- (Ala)₃-NH₂ at 2.5 Å resolution. International

- Seminar-Cum-School on Macromolecular Crystallographic Data, Saha Institute of Nuclear Physics, Calcutta, 16-20 November 1995.
- 1995 **Saxena, A. K.** and Singh, T. P.; X-ray structure determination of the complexes of Proteinase K and designed peptides. National Symposium on Cellular and Molecular Biophysics, Nizam College, Hyderabad, 11-13 January 1995.
- 1993 **Saxena, A. K.**, Singh, T. P., Betzel, Ch., Visanji, M., Peters, K. and Fittkau, S.; Structure of a ternary complex of proteinase K, Hg²⁺ and substrate - analogue Hexapeptide N-Ac-Pro-Ala-Pro-Phe-Pro-Ala-NH₂ at 2.2 Å resolution. XVIth IUCr Congress and General Assembly, International Union of Crystallography, Beijing, 21-29 August 1993.
- 1993 **A. K. Saxena**, P. Sharma, A. Srinivasan and T. P. Singh; Design and synthesis of a chymotrypsin inhibitor N-Ac-dehydro-Phe-Az lactone, its structure and complex formation with chymotrypsin. National Symposium on Molecular and Cellular Biophysics, Anantpur, Hyderabad, 7-9 January 1993.
- 1993 Workshop on "Fundamental of Computer Modelling of Biomolecular Interaction" held at All India Institute of Medical Sciences, Delhi, 26-29 April 1993.
- 1992 **Saxena, A. K.**, Sharma, P., Srinivasan, A., Rao, G. S. & Singh, T. P.; Structure of N-Acdehydro-Phe-L-Val-OH/OCH₃ in different solvents such as Benzene, Acetonitrile, Ethylacetate, DMSO, Chloroform, Methanol and theoretical conformational calculation using different dielectric constants. XXIV National Seminar on Crystallography and Microsymposium on the Crystallography of Superconducting Materials, Jammu, 20-22 October 1992.
- 1992 **Saxena, A. K.**, Dey, S., Sharma, P., Khandelwal, B., Rao, G. S. & Singh, T. P.; Conformation of peptide N-Ac-dehydro-Phe-L-Val-OH in Acetonitrile and Benzene and Synthesis of Chymotrypsin Inhibitor by incorporating dehydro-Phe, its structure and complex formation with Chymotrpsin. XXII National Seminar on Crystallography, Department of Physics, Malviya Regional Engineering College, Jaipur, 23-25 March 1992.
- 1992 Workshop/ Training programmes of Single Crystal X-ray diffractometer held at All India Institute of Medical Sciences, Delhi, 6-12 April 1992.
- 1990 **Saxena, A. K.**, Sinha, S. K. and Singh, T. P. ; Synthesis, Crystal structure and Molecular conformation of 1-Formyl-3-Thiosemicarbazide. XXII National Seminar on Crystallography, Indian Association for Cultivation of Science, Jadavpur, Calcutta, 26-28 December 1990. This paper has been adjudged best in the poster session.