

## CURRICULUM VITAE

Prof. Ajay Kumar Saxena  
Structural Biology Lab  
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### Education:

1990-1995 Ph.D. in Structural Biology (Protein Crystallography), AIIMS, 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, Maryland, USA  
1996-1998 Postdoctoral Fellow, Institute of Biophysics & X-ray Structure Research, Austrian Academy of Sciences, Austria, Europe

### Awards/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:

2018-2023 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+CFP10/ESAT6 complex from ESX-1 virulence factor 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*  
2010-2013 Department of Science and Technology (DST), India.

- 2011-2014 Project- Structural and functional analysis of **ERG** oncoprotein: potential target to develop prostate cancer drug. *PI-Ajay K. Saxena*  
Council of Scientific and Industrial Research (CSIR), India.
- 2006-2009 Project-Structure analysis of *M. tuberculosis* **CarD** protein: an essential regulator of rRNA transcription. *PI-Ajay K. Saxena*  
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

#### Memberships of professional Societies:

- American crystallographic association
- European crystallographic association
- Asian crystallographic association

#### Adhoc reviewer:

- Nature Commun., PLoS One, BMC crystallography, Sci. Rep., Protein Science, IUCr journals

#### Undergraduate teaching

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

#### Administrative Positions/Activities

- Member-House allotment committee (2018-2020)
- Member-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)
- 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

- Concurrent faculty-School of Sanskrit (2019-2021)
- External member, School of System Medicine, JNU (2021- )
- Proctor, Jawaharlal Nehru University (2019-2021)

- Academic Committee Member, IMTECH, Chandigarh, India (2019- 2021)
- Academic Committee Member, NII, New Delhi, India (2017- 2019)
- Academic Committee Member, CCMB, Hyderabad, India (2018- 2020)
- Academic Council Member, JNU, New Delhi (Feb 19, 2020-2022)
- LEAP Program participant at JNU, New Delhi and NUS at Singapore (Feb 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

#### No. of Ph. D./M. tech/MS

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

## RESEARCH ACCOMPLISHMENTS

### Project 1. Structure-function analysis of *M. tuberculosis* drug/vaccine candidate proteins

The ESX-1 secretion system of *M. tuberculosis* delivers bacterial proteins into host cell during mycobacterial infection. The structure-function analysis of the protein will contribute significantly in designing therapeutics against *M. tuberculosis* disease.

#### P1. *M. tuberculosis* (i) Rv3868+EspC complex (ii) Rv3870+ Rv3871+ ESAT6 /CFP10 complex (iii) EspR regulator

In current project, we have structurally and functionally characterized the Rv3868 and Rv3870+Rv3871 of ESX-1 section system and their complexes with EspC and ESAT6/CFP10 virulence proteins.

#### P2. *M. tuberculosis* (i) GmhA/HddA/GimB (ii) DprE1/E2 enzymes involved in cell wall biogenesis

In current project, we have determined the low-resolution structure using SAXS, kinetic structurally and functionally characterized all enzymes (GmhA, HddA and GmhB) involved in GDP-heptose biosynthetic pathway and looking forward for specific inhibitor/drug development.

#### P3. *M. tuberculosis* (i) Rv0081/MprA/MprB transcription factors (iii) CarD/RNAP complex from stress regulatory system

In current project, we have structural and functionally characterized various transcription factors involved in ESX-1 regulation, stress regulation and dormant stage of mycobacteria. (1) Gangwar et al., 2011, *Acta Cryst, F*, F67, 83-86 (2) Gangwar et al., 2014, *Acta Cryst F*, F70, 433-437 (3) Gangwar et al., *Acta Cryst F70* (2014) 160-165 (4) Meena et al., 2016, *J. Phys. Chem. Biophys.* 6:3 (5) Karan et al., 2017, *J. Mol. Model* 23:241 (6) Karan et al., 2019, *Int. J. Biol. Macromol* 136 (2019) 676–685 (7) Karan et al., 2020, *Scientific Report* (8) Gangwar et al., *bioRxiv preprint*, 2020 (9) Karan et al., 2021, *Int. J. Biol. Macromol* 171 (28-36) (10) Arkita et al., 2021, *Int. J. Biol. Macromol* 189: 879–889.

**Project 2. Structure-function analysis 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 project, we are focusing on structural and biochemical studies on following vaccine candidate proteins,

**P1. 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.

(1) Saxena et. al., *Acta Cryst D* 60 2054, 2004 (2) Saxena et. al., *Cryst D* 60 706, 2004 (3) Saxena et. al., (*Struc. & Mol. Biol*) 13(1), 2006 (4) Saxena et. al., *Eukar. Cell*, 6(8), 2007 (5) Sharma et. al., *J. Mol. Model.* 15(4), 2009 (6) Sharma et. al., *J. Mol. Model.* 15(3), 2009 (7) Saxena et. al., *Int. J. Biol. Macromol.* 50, 2012.

**P2. Plasmodium cysteine proteases (i) Falcipain and (iii) Metacaspase-2/ 3 enzymes.**

In current project, we have functionally and structurally characterized the *Plasmodium* Falcipain-2/Falcipain-3 and Metacaspase-2/Metacaspase-3 enzymes

(1) Sudararaj et. al., 2012, *PLoS ONE*, 7(10) (2) Sudararaj et. al., 2014, *PLoS ONE*, 9(4) (3) Vandana et. al., 2018, *Molecular & Biochemical Parasitology* 220: 28–41 (4) Ahuja et. al., 2018, *BBA-Molecular Cell Research* 1865(8): 1148-1159 (5) Pant et. al., 2018, *Sci. Rep.* 8:16193 (6) Pasupureddy et. al., 2019, *Experimental Parasitology* 197:43-50 (7) Bhumika et. al., 2019, *Int. J. Biol. Macromol.* 138: 309-320 (8) Vandana et. al., 2021, *The Journal of Biochemistry*

**Project 3. Structure-function analysis of cancer related proteins**

In cancer project, we have expressed, purified, biochemically characterized and solve the x-ray structure of Ergp55-DNA complex. Ergp55 is the most frequent proto-oncogenic alterations in prostate cancer cell and directly involved in prostate cancer. In research projects, we have crystallized and determined the X-ray structure of membrane yeast Sac1, Cdr1p and TAP proteins.

**P1. Human antigenic peptide transporter TAP**

**P2. C. albicans Cdr1p multidrug transporter, Yeast Sac-1 enzyme**

**P3. Human Ergp55 oncoprotein**

(1) Manford et. al., 2010, *The EMBO Journal* 29, 1489–1498 (2) Gangwar et. al., 2011, *Acta Cryst. F* 68, 83-86 (3) Gangwar et. al., 2012, *PLoS ONE* 7(6), e39850 (4) Meena et. al., 2012, *Acta Crystallogr. Section F Biol. Crystallogr.* F68, 655–658 (5) Rawal et. al., 2013, *J. Biol. Chem.* 288(34), 24480-93 (6) Shah et. al., 2015, *Sci. Rep.*, 2015, 5:11211 (7) Shah et. al., 2015 *FEMS Yeast Res.* 15(5). pii: fov036 (8) Rawal et. al., 2016, *Sci. Rep.* 6:27132 (9) Sharma et. al., 2018, *Acta Crystallogr. Section F Biol. Crystallogr.* F74, 656-663 (10) Sukrit et. al., 2020, *J. Biomol. Struc. & Dynamics*, DOI: 10.1080/07391102.2020.1838329 (11) Sukrit et. al., *JMIR Bioinformatics Biotechnol* 2020 1(1): e19371 (12) Sukrit et. al., 2019, *J. Biomol. Struc. & Dynamics*, 37(16): 4345–4360 (13) Sukrit et. al., 2018, *Infection and Drug Resistance* 11: 1–15. (14) Jawa et. al., 2021, *Front. Oncol.* 11:676948.

## PUBLICATIONS (# corresponding author)

2021

55. Sukrit Srivastava, **Ajay Kumar 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 preprint doi: <https://doi.org/10.1101/2021.09.17.460735>*
54. 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.*
53. 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.*
52. 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>.*
51. 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 non-canonical way. *The journal of Biochemistry mvab086*, <https://doi.org/10.1093/jb/mvab086>
50. Sumita Karan, Ankita Behl, Amin Sagar, Arkita Bandhopadhyay, **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.*

2016-2020

49. 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):20813.*
48. S. P. Gangwar, A. Bandyopadhyay and **Ajay K. Saxena#** (2020). Structural studies on *M. tuberculosis* decaprenyl phosphoryl- $\beta$ -Dribose epimerase-2 enzyme involved in cell wall biogenesis. *bioRxiv preprint doi: <https://doi.org/10.1101/2020.10.15.341941>*
47. S. Srivastava, S. Verma, M. Kamthania , D. Agarwal , **Ajay K. Saxena** , M. Kolbe , S. Singh , A. Kotnis , B. Rathi , S. A. Nayar , H-J Shin , K. Vashisht & K. C. Pandey (2020). Computationally validated SARS-CoV-2 CTL and HTL Multi-Patch vaccines, designed by reverseepitomics approach, show potential to coverlarge ethnically distributed human population worldwide, *Journal of Biomolecular Structure and Dynamics, DOI: 10.1080 /07391102.2020.1838329*

46. Srivastava, S., Verma, S., Kamthania, M., Kaur, R., Badyal, R.K., **Saxena, A. K.**, Shin, H.J., Kolbe, M. and Pandey, K.C. (2020). Structural basis to design multi-epitope vaccines against Novel Coronavirus 19 (COVID19) infection, the ongoing pandemic emergency: an in-silico approach.  
*JMIR Bioinformatics Biotechnol* 2020 1(1): e19371.
45. Srivastava, S., Kamthania, M., Kumar Pandey, Kumar R., **Saxena, A. K.**, Saxena, V., Kumar Singh, S., Kumar Sharma, R. and Sharma, N. (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.
44. 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.
43. 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.
42. 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.
41. 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: 16193.
40. S. Srivastava, M. Kamthania, **A. K Saxena**, N. Sharma (2018). *In silico* approach to develop a Multi-Epitope Vaccines against MERS Coronavirus satisfying human HLA, TAP and TLR-3 checkpoints  
*Infection and Drug Resistance* 11: 1–15.
39. 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.* F74: 656-663.
38. K. Ahuja, M. A. Beg, R. Sharma, **A. K. Saxena**, N. Naqvi, N. Puri, A. Chaudhury, R. Duncan, P. Salotra, H. Nakhasi, A. Selvapandiyan (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.
37. Vandana, A. P. Singh, J. Singh, R. Sharma, M. Akhter, P. K. Mishrag, **A. K. Saxena**, R. Dixit, B. Rathie, A. Katyalf, K. C. Pandey (2018). Biochemical characterization of unusual cysteine protease of *P. falciparum*, metacaspase-2 (MCA-2)  
*Molecular & Biochemical Parasitology* 220: 28–41.

36. 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.* 23:241.
35. 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.
34. S. R. Meena and **A. K. Saxena#** (2016). Structure of *E. coli* **GroEL** in substate and ADP unloaded state (**PDB-4HEL**)  
*J. Phys. Chem. Biophys.* 6:3

## 2011-2015

33. 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 intracel- lular loop and nucleotide-binding domain important for protein trafficking.  
*FEMS Yeast Res.* 15(5). pii: fov036.
32. 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: 11211.
31. 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.
30. S. P. Gangwar, S. R. Meena and **A. K. Saxena#**(2014). Comparison of differ- ent crystal forms of ESX-1 secreted protein regulator **EspR** from *M. tuberculo- sis* and its implication for protein regulator activity (**PDB-4NDW**)  
*Acta Crystallogr. Section F Biol. Crystallogr.* F70, 433-437.
29. 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.* F70, 160-165.
28. 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),2448093.
27. 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.

26. 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): e7227.
25. **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.
24. 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.* F68, 655-658.
23. 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.* F68, 1333-1336.
22. **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)
21. 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.* F67, 83-86.
20. **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

19. 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.
18. 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.
17. Sharma B., Jaiswal M. K. and **Saxena, A. K.#** (2009). EGF domain II of protein **Pb28** from *P. berghei* interacts with monoclonal transmission blocking antibody 13.1. *J. Mol. Model* 15(4), 369-382.
16. **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.



15. **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.
14. 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

13. **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.* D60, 2054-2057.
12. **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.* D60, 706-708.

#### 1996-2000

11. **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.* D54, 1450-1452.
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-NH<sub>2</sub> 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)<sub>3</sub>-NH<sub>2</sub> at 2.5 Å resolution (**PDB-1PFG**). *Protein Science* 5, 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.

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/OCH<sub>3</sub> 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)(PPh<sub>3</sub>)<sub>2</sub>]. *Polyhedron* 14, 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, 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**, Hg<sup>2+</sup> and substrate analogue hexpeptide N-Ac-Pro-Ala-Pro-Phe-Pro-Ala-NH<sub>2</sub>. *Acta Crystallogr.* A49 (Supplement), C106.
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CONFERENCE PAPERS (100)

- 2021 **Saxena A. K. (2021)** Workshop on “*Strategy for future EMBL research in the Life Sciences in Hamburg*, March 29, Hamburg, Germany.
- 2021 **Saxena, A. K. (2021)** *14<sup>th</sup> International Symposium on Cancer Prevention and Therapeutics*, Jawaharlal Nehru University, March 16-17, New Delhi, India.
- 2020 Arkita Bandyopadhyay 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). *46<sup>th</sup> 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. 3<sup>rd</sup> Poster Presentation (EBS - 19) 86<sup>th</sup> 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 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 56<sup>th</sup> Association of Microbiologists of India (AMI)* 8-10<sup>th</sup> December, 2015, Jawaharlal Nehru University, New Delhi.
- 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 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.
- 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 Associated 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)<sub>3</sub>-NH<sub>2</sub> 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.
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- 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/OCH<sub>3</sub> 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.