CURRICULUM VITAE

NAME: Dr. Pravindra Kumar, Professor

Department of Biotechnology

Indian Institute of Technology Roorkee, Roorkee – 247 667 Phone: +91-01332-285072 (office), 91-01332-285803 (Res)

Fax: +91-01332-273560 Email: kumarfbs@iitr.ac.in

Area of Specialization: Structural biology

Academic qualification:

Degree	Subject	University/ Institution	Year	Percentage of marks & Class/
				Grade
B.Sc.	Physics, Chemistry, Maths	Meerut University	1993	First Class
M.Sc.	Physics	C.C.S. Uni. Meerut	1995	First Class
Ph.D.	Biophysics	A.I.I.M.S. Delhi	2001	Best Ph.D. award (Gold medal)

Ph. D. (Biophysics): All India Institute of Medical Sciences,. New Delhi 1996-2001

Title: "Three Dimensional Structure Determination of Lactoferrin." Gold Medal for Best Ph.D. .

Teaching & Research Experience:

Position	University/ Institution	Dates
Professor	Indian Institute of Technology, Roorkee	Dec 22, 2018-Present
Associate Professor	Indian Institute of Technology, Roorkee	Oct 23, 2012-Dec 21, 2018
ASM Visiting Professor by Indo-US forum (IUSSTF)	Purdue University, USA	May-July 2017
Boyscast Fellow, DST-Govt. of India	Purdue University, USA	May-Sep 2008
Visiting Professor	Purdue University, USA	May-July 2006
Assistant Professor	Indian Institute of Technology, Roorkee	2005-2012
Post-Doc	Purdue University, USA	2001-2005
Senior Research Fellow (C.S.I.R. SRF)	A.I.I.M.S. New Delhi, India	1999-2001

Senior Demonstrator	A.I.I.M.S.New Delhi, India	1996-1999

Awards and Recognition's:

- 1. ASM-IUSSTF INDO-US Visiting Professorship, 2017
- 2. National Bioscience Award in 2016 by DBT, Ministry of Science & Technology, Govt. of India.
- 3. IUSSTF Award 2014 for organizing Indo-US conference and Symposium 2014
- 4. BOYSCAST award (2008) from Department of Science and Technology, India and Visiting Scientist to USA
- 5. Visiting Scientist (May-July 2006) at Purdue University, USA
- 6. Senior Research Fellowship, Council of Scientific and Industrial Research (1999-2001)
- 7. S.V. TALEKAR MEDAL for Best Post Graduate Degree in AIIMS, DELHI

Theses/Dissertation supervised:

Ph.D. Thesis: 13 Awarded; 01 submitted and 06 in progress

M.Sc. Dissertation: 22 completed; 01 in progress

Ph. D. Supervised:

SNo.	Title	Year	Name of Scholar	Co-Supervisor
		Awarded		(if any)
1.	Structural And Functional Studies Of Plant Proteins	Submitted	Pooja Kesari	-
2.	Structural And Biochemical Characterization Of Protein Drug Targets From Human Pathogens	Nov 2018	Madhusudhanarao Katiki	-
3.	Biophysical, Biochemical And Structural Characterization Of Drug Targets From Bacteria	July 2018	Anchal Sharma	-
4.	Xenobiotic Compounds Degradation And Their Effects On Important Enzymes	June 2018	Neha Singh	-
5.	Structural Sudies Of Shikimate And Fatty Acid Biosynthesis Pathway's Enzymes	Mar 2018	Vijay Kumar	-
6.	Studies On Peroxyredoxin Antioxidant System From Candidatus Liberibacter asiaticus	Sep 2015	Anamika Singh	Dr. A.K. Sharma
7.	Structural Studies Of Enzymes Involved In Bioremediation	Oct 2014	Sonali Dhindwal	Dr. S. Tomar
8.	Structural Studies On 11s Globulin And 2s Albumin From Wrightia tinctoria	March 2014	Pramod Kumar	Dr. B.R. Gurjar
9.	Structural Characterization Of Drug Targets	Dec 2013	Shivendra Pratap	-

	From Drug Resistant Pathogenic Bacteria			
10.	Structural Studies On Mura And Type II Chorismate Mutase	Dec 2013	Aditya Dev	Dr. Shishir Sinha
11.	Structure-Function Studies On Miraculin- Like Proteins	Dec 2012	P. Selvakumar	Dr. A.K. Sharma
12.	Structural Studies Of Protease Inhibitor Complex And Chitinase Like Lectin From Tamarind	May 2012	Dipak N. Patil	-
13.	Structural Characterization Of Chitinase	May 2009	Manali Datta	Dr. A.K. Sharma
14.	Structural Studies On Some Metalloproteins: Biphenyl Dioxygenase And DAHP Synthase	Feb 2009	Sushmita Bhattacharya	-

Ph. D. On-going:

Scholar Name	Interest
Ms. Vishakha Singh	Structural studies of bacterial enzymes involved in bioremediation of
	plastics
Ms. Monica Sharma	Computational Biology of proteins involved in bioremediation
Mr. Jaikrishna	Structural characterization of enzymes involved in bioremediation of
	phthalates
Ms. Poonam Dhanakar	Structural biology of dye-degrading bacterial enzymes
Mr. Vikram Dalal	Structural studies of new drug targets from bacteria
Ms. Neetu	Structural characterization of enzymes of shikimate pathway

<u>Details of Sponsored Research Projects as PI:</u>

S.No	Title	Sponsoring	Co-PI	Duration	Amo
		Agency			unt
					(in
					lakh)
1.	Structural Studies of Aromatic-ring- Hydroxylating Dioxygenasees and their complexes with toxic Polyaromatic compounds	DST	-	2006-2008	11.16
2.	Structural characterization of the enzymes involved in the biodegradation of polychlorinated biphenyls and other Waste materials	MHRD- IITR	-	2006	1.0
3.	Structural studies of biphenyl dehydrogenase from <i>Comamonas</i>	C.S.I.R.	Dr. Shailly Tomar, Dr.	2008-2011	10.7

	testosteroni strain B-356		AK. Sharma		
4.	Structural Characterization Of DAHP Synthase For Designing Rational Inhibitors As Antibacterial Drug.	MHRD- SCHEME- B	Dr. Shailly Tomar, Dr. AK. Sharma	2008-2011	9.6
5.	Structural analysis of DAHP synthase from <i>Arabidopsis thaliana</i>	DST	Dr. Shailly Tomar, Dr. AK. Sharma	2010-2013	29.95
6.	Microbial degradation of toxic aromatic compounds using structural biology approach.	DRDO	Nil	2012-2015	41.27
7.	Structure-based development of anti- bacterial enzyme inhibitors against enzyme involved in lipooligosaccharide(LOS) biosynthesis: Structure determination and in-silico drug design against Moraxella catarrhalisUDP-N-acetylglucosamine acyltransferase (LpxA)	ICMR	Nil	2012-2015	40.0
8.	Structural studies of chorismate synthase	CSIR	Dr. Shailly Tomar, Dr. AK. Sharma	2013-2016	23.0
9.	Structural studies of 11s Globulin from Wrightia Tinctoria, a medical plant	DBT	Dr. Shailly Tomar, Dr. AK. Sharma	2014-2017	26.0
10.	Structure based inhibitors an enzymes: UDP-n-acetylglucosamine- carboxyvinyltransferase (murA) from Provindencia Alcalifaciens	DRDO	Dr. Harsh	2016-2019	9.5
11.	Structural characterization of Moraxella Catarrhalis enoylacyl carrier protein reductase (FabI) and in-silico inhibitor	ICMR	Nil	2015-2018	40.0
12.	Biodegradation of phthalates	DBT	Nil	2016-2019	15.0
13.	Structural characterization of dye- decoiorizing peroxidase enzyme from Bacillus Subtilis and Pseudomonas Putida with an aim for bioremediation of industrial wastewater	DBT	Prof. Bhola Ram Gurjar, Dr. A.K. Sharma	2017-2020	40.0

<u>Details of Sponsored Research Projects as Co- PI:</u>

S.No	Title	Sponsoring	PI	Duration	Amount
		Agency			(in lakh)

1.	Structural functional studies of alphavirus nsP1	DST	Dr. Shailly Tomar	2006-2009	8.6
2.	Structural studies of tamarind proteinase inhibitor (TPI) and its complex with trypsin.	CSIR	Dr. Shailly Tomar	2010-2013	15.76
3.	Structural analysis of chitinase from Tamarindus indica	DST	Dr. Shailly Tomar	2013-2016	37.34
4.	In silico development of anti-amoebic molecules based on the structure of E. histolytica ornithine decarboxylase	ICMR	Dr. Shailly Tomar	2015-2018	49.92
5.	Structural functional characterization of Chikungunya virus nsP2 protease and protease inhibitor screening	DBT	Dr. Shailly Tomar	2014-2018	50.0
6.	Probing molecular contacts between capsid protein and envelop proteins of Chikungunya Virus	ICMR	Dr. Shailly Tomar	2017-2020	49.9
7.	Structure analysis of a trypsin inhibitor purified from seeds of <i>Murraya koenigii</i>	DST	Dr. A.K. Sharma	2008-2011	19.92
8.	Structure-function studies of a trypsin inhibitor purified from seeds of <i>Putranjiva roxburghii</i> .	CSIR	Dr. A.K. Sharma	2009-2012	14.26

Publication list

2018

- 1. Kaur R, Neetu, Mudgal R, Jose J, Kumar P, Tomar S. (2019) Glycan-dependent chikungunya viral infection divulged by antiviral activity of NAG specific chi-like lectin. *Virology* 2;526:91-98. **Neetu is pursuing her PhD with Kumar, P; Kaur R, Mudgal R are pursuing her PhD with Tomar S; Jose J and Kumar, P are collaborators.**
- 2. Kumar V, Sharma A, Pratap S, **Kumar**, **P***. Biochemical and biophysical characterization of 1,4-Naphthoquinone as a dual inhibitor of two key enzymes of type II fatty acid biosynthesis from Moraxella catarrhalis. (*Biochim Biophys Acta. Protein and Proteomics*) 1866(11):1131-1142...

Kumar V, Sharma A, Pratap S did their PhD with Kumar, P.(*Corresponding author)

- 3. Narwal M, Singh H, Pratap S, Malik A, Kuhn RJ, **Kumar**, **P**, Tomar S. Crystal structure of chikungunya virus nsP2 cysteine protease reveals a putative flexible loop blocking its active site. *Int J Biol Macromol*. (2018); 116:451-462. PubMed PMID: 29730006.
 - Pratap S did PhD with Kumar, P; Tomar S and Kuhn RJ are collaborators, Narwal M, Singh H, Malik A are pursuing her PhD with Tomar S.
- 4. Sharma A, Kumar V, Pratap S, **Kumar**, **P***. The inhibitory and binding studies of methyl-sulfone hydroxamate based inhibitors against LpxC from drug resistant *Moraxella catarrhalis* using biophysical, biochemical and in silico approaches. *Int J Biol Macromol*. (2018). PubMed PMID: 30017978.

- 5. Kumar V, Sharma A, Pratap S, **Kumar, P***. Biophysical and in silico interaction studies of aporphine alkaloids with Malonyl-CoA: ACP transacylase (FabD) from drug resistant Moraxella catarrhalis. *Biochimie*. (2018); 149:18-33. PubMed PMID: 29604333.
 - Kumar V, Sharma A, Pratap S did their PhD with Kumar, P. (*Corresponding author)
- Kumar V, Sharma A, Pratap S, Kumar, P*. Characterization of isoflavonoids as inhibitors of β-hydroxyacyl-acyl carrier protein dehydratase (FabZ) from Moraxella catarrhalis: Kinetics, spectroscopic, thermodynamics and in silico studies. *Biochim Biophys Acta*. (2018); 1862(3):726-744. PubMed PMID: 29092780.
 - Kumar V, Sharma A, Pratap S did their PhD with Kumar, P. (*Corresponding author)
- 7. Sharma R, Kesari P, **Kumar**, **P**, Tomar S. Structure-function insights into chikungunya virus capsid protein: Small molecules targeting capsid hydrophobic pocket. *Virology* (2018); 515:223-234.
 - Kesari P is a PhD student of Kumar, P; Sharma R did his PhD with Tomar S, a faculty colleague.
- 8. Singh N, Dalal V, **Kumar**, **P***. Structure based mimicking of Phthalic acid esters (PAEs) and inhibition of hACMSD, an important enzyme of the tryptophan kynurenine metabolism pathway. *Int J Biol Macromol*. (2018); 108:214-224.
 - Singh N, Dalal V are PhD students of Kumar, P. (*Corresponding author)
- Kumar V, Sharma A, Pratap S, Kumar, P*. Characterization of isoflavonoids as inhibitors of β-hydroxyacyl-acyl carrier protein dehydratase (FabZ) from Moraxella catarrhalis: Kinetics, spectroscopic, thermodynamics and in silico studies. *Biochim Biophys Acta*. (General Subjects) (2018); 1862(3):726-744.
 - Kumar V, Sharma A, Pratap S did their PhD with Kumar, P. (*Corresponding author)
- 10. Sharma A, Kumar V, Chatrath A, Dev A, Prasad R, Sharma AK, Tomar S, **Kumar**, **P*** In vitro metal catalyzed oxidative stress in DAH7PS: Methionine modification leads to structure destabilization and induce amorphous aggregation. *Int J Biol Macromol*. (2018);106:1089-1106
 - Sharma a, Kumar V, Dev a did their PhD with Kumar, P; Chatrath a is PhD students of Prasad R; Prasad R, Sharma AK and Tomar S are faculty colleagues. (*Corresponding author)

- 1. Aggarwal M, Kaur R, Saha A, Mudgal R, Yadav R, Dash PK, Parida M, **Kumar**, **P**, Tomar S. Evaluation of antiviral activity of piperazine against Chikungunya virus targeting hydrophobic pocket of alphavirus capsid protein. *Antiviral Res.* (2017);146:102-111.
 - Yadav R was project student with Kumar, P; Tomar S is a faculty colleague, Dash PK and Parida M are collaborator, Aggarwal M, Kaur R, Mudgal R, are PhD students of Tomar S.
- 2. Pratap S, Dev A, Kumar V, Yadav R, Narwal M, Tomar S, **Kumar, P***. Structure of Chorismate Mutase-like Domain of DAHPS from Bacillus subtilis Complexed with Novel Inhibitor Reveals Conformational Plasticity of Active Site. Nature Publishing group *Sci Rep.* (2017); 25;7(1):6364.
 - Pratap S, Dev A, Kumar V did their PhD and Yadav R did B Tech and was project student with Kumar, P; Narwal M did her PhD with Tomar S, faculty colleague. (*Corresponding author)

- 3. Kumar, P, Kesari P, Dhindwal S, Choudhary AK, Katiki M, Neetu, Verma A, Ambatipudi K, Tomar S, Sharma AK, Mishra G, **Kumar**, **P***. A novel function for globulin in sequestering plant hormone: Crystal structure of Wrightia tinctoria 11S globulin in complex with auxin. Nature Publishing group *Sci Rep*. (Nature Publishing Journal) (2017); 7(1):4705. **Kumar**, **P**, **Kesari P**, **Dhindwal S**, **Katiki M**, **Neetu are PhD students of Kumar**, **P**; **Choudhary AK is PhD student of Mishra G**; **Verma A is PhD student of Ambatipudi K**; **Ambatipudi K**, **Tomar S and Sharma AK are faculty colleagues**; **Mishra G is a collaborator**. (*Corresponding author)
- 4. Singh N, Dalal V, Mahto JK, **Kumar, P***. Biodegradation of phthalic acid esters (PAEs) and in silico structural characterization of mono-2-ethylhexyl phthalate (MEHP) hydrolase on the basis of close structural homolog. *J Hazard Mater*. (2017); 15;338:11-22. **Singh N, Dalal V, Mahto JK are PhD students of Kumar, P.** (*Corresponding author)
- Kesari P, Neetu, Sharma A, Katiki M, Kumar, P, Gurjar BR, Tomar S, Sharma AK, Kumar, P*. Structural, Functional and Evolutionary Aspects of Seed Globulins. *Protein Pept Lett.* (2017); 24(3):267-277.
 Kesari P, Neetu, Sharma A, Katiki M, Kumar, P are PhD students of Kumar, P; Gurjar
 - Kesari P, Neetu, Sharma A, Katiki M, Kumar, P are PhD students of Kumar, P; Gurjar BR, Tomar S and Sharma AK are faculty colleagues. (*Corresponding author)
- 6. Sharma A, Kumar, P, Kesari P, Chaudhary N, Katiki M, Mishra M, Singh PK, Gurjar, BR, Sharma AK, Tomar S, **Kumar**, **P***. Purification and Characterization of 2S albumin from seeds of Wrightia tinctoria exhibiting Antibacterial and DNase Activity. *Protein Pept Lett.* (2017); 24(4):368-378.
 - Sharma A, Kumar, P, Kesari P, Chaudhary N, Katiki M, are PhD students of Kumar, P; Gurjar BR, Tomar S and Sharma AK are faculty colleagues; Mishra M is doing PhD with Singh PK, a collaborator. (*Corresponding author)
- 7. Pratap S, Kesari, P, Yadav R, Dev A, Narwal M & **Kumar, P***. Acyl chain preference and inhibitor identification of Moraxella catarrhalis LpxA: Insight through crystal structure and computational studies. *Int J Biol Macromol*. (2017); 96:759-765.
 - Pratap S, Kesari, P, Dev A, are PhD students and Yadav R is B. Tech student of Kumar, P. Narwal M is a PhD student from collaborative lab. (*Corresponding author)

- 1. Dhindwal S, Gomez-Gil L, Neau DB, Pham TT, Sylvestre M, Eltis LD, Bolin JT, **Kumar**, **P***. The structural basis of the enhanced pollutant-degrading capabilities of an engineered biphenyl dioxygenase. *J Bacteriol*. (2016); 198(10) 1499-512.
 - Dhindwal S did her Phd with Kumar, P. Gomez-Gil L, Neau DB, Pham TT, Sylvestre M, Eltis LD, Bolin JT are collaborators. (*Corresponding author)
- 2. Dhindwal S, Kesari P, Singh H, Kumar, P, Tomar S. Conformer and pharmacophore based identification of peptidomimetic inhibitors of chikungunya virus nsP2 protease. *J Biomol Struct Dyn.* (2017); 35(16):3522-3539.
 - Dhindwal S and Kesari P are PhD students of Kumar, P; Singh H is a PhD student of Tomar S, faculty colleague.

- 3. Sharma R, Fatma B, Saha A, Bajpai S, Sistla S, Dash PK, Parida M, Kumar, P,Tomar S. Inhibition of chikungunya virus by picolinate that targets viral capsid protein. *Virology*. (2016); 498:265-276. PubMed PMID: 27614702.
 - Kumar P helped in 3D structure determination; Sharma R and Fatma B are PhD students of Tomar S, faculty colleague; Saha A is PhD student of Dash PK; Bajpai S, Sistla S, and Parida M are collaborators.
- 4. Batra M, Sharma R, Malik A, Dhindwal S, Kumar, P, Tomar S Crystal structure of pentapeptide-independent chemotaxis receptor methyltransferase (CheR) reveals idiosyncratic structural determinants for receptor recognition *J Struct Biol.* (2016); 196(3):364-374
 - Dhindwal S did her PhD with Kumar, P. Batra M, Sharma R, Malik A are PhD students of Tomar S, a faculty colleague.
- 5. Tomar JS, Narwal M, **Kumar, P**, Peddinti RK. Characterization of substrate binding and enzymatic removal of a 3-methyladenine lesion from genomic DNA with TAG of MDR *A. baumannii*. *Mol Biosyst.* (2016); 12(11):3259-3265. PubMed PMID: 27714027.
 - Kumar, P helped in experiments; Peddinti RK faculty colleague; Tomar JS is student of Peddinti RK.
- 6. Mukhi N, Dhindwal S, Uppal S, Kapoor A, Arya R, Kumar, P, Kaur J, Kundu S. Structural and Functional Significance of the N- and C-Terminal Appendages in Arabidopsis Truncated Hemoglobin. *Biochemistry*.(2016); 55(12):1724-40.
 - Dhindwal S did her PhD with Kumar, P; Kundu S. is a collaborator.

- 1. Pratap S, Katiki M, Gill P, **Kumar, P***, Golemi-Kotra D. (* Corresponding author). Active-Site Plasticity is Essential to Carbapenem Hydrolysis by OXA-58 Class D β-Lactamase of Acinetobacter baumannii. *Antimicrob Agents Chemother*. (2015); 60(1):75-86.
 - Pratap S, Katiki M are PhD students of Kumar, P; Gill P did his PhD with Golemi-Kotra D, a collaborator. .(*Corresponding author)
- 2. Dhindwal S, Priyadarshini P, Patil DN, Tapas S, Kumar, P, Tomar S, **Kumar**, **P***. Ligand-bound structures of 3-deoxy-D-manno octulosonate 8-phosphate phosphatase from Moraxella catarrhalis reveal a water channel connecting the active site for the second step of catalysis. *Acta Crystallogr D Biol Crystallogr*. (2015); 71(Pt 2):239-55.
 - $\begin{array}{l} \textbf{Dhindwal S, Patil DN and Kumar, P did their PhD and Priyadarshini P did Project with Kumar, P; Tapas S did his PhD with Tomar S. .(*Corresponding author)} \end{array}$
- 3. Sharma N, SelvaKumar, P, Bhose S, Ghosh DK, **Kumar**, **P**, Sharma AK. Crystal structure of a periplasmic solute binding protein in metal-free, intermediate and metal-bound states from *Candidatus Liberibacter asiaticus*. *J Struct Biol*. (2015); 189(3):184-94
 - SelvaKumar, P is a PhD student of Kumar, P and Sharma AK; Bhose S, Ghosh DK, and Sharma AK are collaborators.
- 4. Aggarwal M, Sharma R, **Kumar, P**, Parida M, Tomar S. Kinetic characterization of transproteolytic activity of Chikungunya virus capsid protease and development of a FRET-based HTS assay. Nature Publishing group *Sci Rep*. (2015); 5:14753.
 - Kumar P helped in structure analysis; Sharma R and Aggarwal M, are PhD students of Tomar S; Parida M is a collaborator.
- 5. Kesari P, Patil DN, Kumar, P, Tomar S, Sharma AK, **Kumar**, **P***. Structural and functional evolution of chitinase- like-proteins from plants. *Proteomics*. (2015); 15(10):1693-705.
 - Kesari P, Patil DN, Kumar, P are PhD student of Kumar, P; Tomar S are Sharma AK are faculty colleagues. .(*Corresponding author)

1. SelvaKumar, P, Sharma N, Tomar PP, **Kumar**, **P**, Sharma AK Structural insights into the aggregation behavior of Murraya koenigii miraculin-like protein below pH 7.5. *Proteins* (2014); 82(5):830-40.

SelvaKumar, P is a PhD student of Kumar, P and Sharma AK; Sharma N and Tomar PP, did their Phd with Sharma AK.

2. Aggarwal M, Dhindwal S, **Kumar, P**, Kuhn RJ, Tomar S. trans-Protease activity and structural insights into the active form of the alphavirus capsid protease. *J Virol*. (2014); 88(21):12242-53.

Dhindwal S did her PhD with Kumar, P; Aggarwal M did her PhD with Tomar S; Kuhn RJ, is a collaborator.

2013

1. Colbert CL, Agar NY, **Kumar**, **P***, Chakko MN, Sinha SC, Powlowski JB, Eltis LD, Bolin JT. Structural characterization of Pandoraea pnomenusa B-356 biphenyl dioxygenase reveals features of potent polychlorinated biphenyl-degrading enzymes *PLoS One.* (2013); 8(1):e52550 (* **First co-author**)

Structure determination was done by Kumar, P. Colbert CL, Agar NY, Chakko MN, Sinha SC, Powlowski JB, Eltis LD, Bolin JT are collaborators.

2. Patil DN, Datta M, Dev A, Dhindwal S, Singh N, Dasauni P, Kundu S, Sharma AK, Tomar S, **Kumar, P***. Structural Investigation of a Novel N-Acetyl Glucosamine Binding Chi-Lectin Which Reveals Evolutionary Relationship with Class III Chitinases. *PLoS One.* (2013); 23;8(5):e63779.

Patil DN, Datta M, Dev A and Dhindwal S, did their PhD with Kumar, P; Kundu S, Sharma AK, Tomar S, are collaborators. (*Corresponding author)

3. Mukhi N, Dhindwal S, Uppal S, **Kumar, P**, Kaur J, Kundu S. X-Ray crystallographic structural characteristics of Arabidopsis hemoglobin I and their functional implications. *Biochim Biophys Acta*. (2013); 1834(9):1944-56.

Dhindwal S did her PhD with Kumar, P; Kundu S. is a collaborator.

4. Preeti, Tapas S, **Kumar, P**, Madhubala R, Tomar S. Structural insight into DFMO resistant ornithine decarboxylase from Entamoeba histolytica: an inkling to adaptive evolution. *PLoS One*.(2013); 8(1):e53397.

Kumar P helped in structure analysis; Preeti and Tapas S, are PhD students of Tomar S, faculty colleague; Madhubala R, is a collaborator.

5. Aggarwal M, Tapas S, Preeti, Siwach A, **Kumar, P**, Kuhn RJ, Tomar S. Crystal structure of aura virus capsid protease and its complex with dioxane: new insights into capsid-glycoprotein molecular contacts. *PLoS One*.(2013); 7(12):e51288.

Kumar P helped in structure analysis; Aggarwal M, Tapas S, Preeti, are PhD students and Siwach A, did project with Tomar S, faculty colleague; Kuhn RJ, is a collaborator.

2012

1. Patil, D.N., Chaudhry, A., Sharma, A.K., Tomar, S., **Kumar, P***. Structural basis for dual inhibitory role of tamarind Kunitz inhibitor (TKI) against factor Xa and trypsin. *FEBS J* (2012); 279(24):4547-64.

Patil, D.N. did his PhD and Chaudhry, A. did Project with Kumar, P; Sharma, A.K. and Tomar, S. are faculty collegues. (*Corresponding author)

2. **Kumar, P**, Mohammadi M, Dhindwal S., Bolin JT &Sylvestre M. Structural insights into the metabolism of 2-chlorodibenzofuran by an evolved biphenyl dioxygenase *BBRC* (2012); 421(4):757-62.

Dhindwal S. did her PhD with Kumar, P; Mohammadi M, Bolin JT &Sylvestre M are collaborators.

- 3. Kumar, P., Patil, D.N., Chaudhary, A., Tomar, S., Yernool, D., Singh, N., Dasauni, P., Kundu, S., & **Kumar**, **P***., Purification and biophysical characterization of 11S globulin from Wrightia tinctoria exhibiting hemagglutinating activity. *Protein & peptide letters* (2012); 20(5):499-509.
 - Kumar, P., Patil, D.N., did their PhD and Chaudhary, A. did project with Kumar, P; Tomar, S., Yernool, D., Singh, N., Dasauni, P., Kundu, S. are collaborators.(*Corresponding author)
- 4. Preeti, Tapas S, **Kumar**, **P**, Madhubala R, Tomar S. Biochemical, Mutational and In Silico Structural Evidence for Functional Dimeric Form of the Ornithine Decarboxylase from Entamoeba histolytica. *PLoSNegl Trop Dis.* (2012); 6(2):e1559.
 - Kumar P helped in structure analysis; Tapas S, Preeti, are PhD students of Tomar S, faculty colleague; Madhubala R, is a collaborator.
- 5. Narayanan A, Paul LN, Tomar S, Patil DN, **Kumar**, **P**, Yernool DA. Structure-function studies of DNA binding domain of response regulator KdpE reveals equal affinity interactions at DNA half-sites. *PLoS One*.(2012); 7(1):e30102.
 - Patil DN did his PhD with Kumar, P; Narayanan A and Paul LN work with Yernool DA, a collaborator; Tomar S is a faculty colleague.

- 1. Dhindwal S, Patil DN, Mohammadi M, Sylvestre M, Tomar S, **Kumar, P*.** Biochemical studies and ligand-bound structures of biphenyl dehydrogenase from Pandoraea pnomenusa strain B-356 reveal a basis for broad specificity of the enzyme. *J Biol Chem.* (2011); Oct 21;286(42):37011-22.
 - **Dhindwal S, Patil DN did their PhD with Kumar, P;** Mohammadi M, Sylvestre M, Tomar S are collaborators. .(*Corresponding author)
- 2. Mohammadi, M.†, Viger, J.F.,†, **Kumar, P.**,†, Barriault, D., Bolin, J.T., &Sylvestre, M. (†Contributed equally). a. Fine tuning Rieske -type oxygenases reactive atoms to expand their substrate range. *J. Biol. Chem.* (2011); 286(31):27612-35.
 - Kumar, P did crystallization and structure studies; Mohammadi, M., Viger, J.F., Barriault, D., Bolin J.T. & Sylvestre M. are collaborators
- 3. **Kumar, P.,** Mohammadi, M., Viger, J.F., Barriault, D., Gomez-Gil, L., Eltis, LD., Bolin J.T. &Sylvestre M. Structural Insight into the Expanded PCB-Degrading Abilities of a Biphenyl Dioxygenase Obtained by Directed Evolution. *J Mol Biol.* (2011); 405(2):531-47.
 - Kumar, P did crystallization and structure studies; Mohammadi, M., Viger, J.F., Barriault, D., Gomez-Gil, L., Eltis, LD., Bolin J.T. &Sylvestre M. are collaborators
- 4. Aggarwal, M., Dhindwal, S., Pratap, S., Kuhn, R.J., **Kumar, P.**,& Tomar, S.Crystallization, high- resolution data collection and preliminary crystallographic analysis of Aura virus capsid protease and its complex with dioxane. *Acta Cryst. F* (2011); 67, 1394-1398. **Dhindwal, S., Pratap, S.,** did **their PhD with Kumar, P**
- 5. Bhattacharya, S., & **Kumar**, **P**. An insilico approach to structural elucidation of 3-deoxy-d arabino-heptulosonate 7-phosphate synthase from Arabidopsis thaliana: Hints for herbicide design. *Phytochemistry*. (2011); 73(1):7-14.
 - Bhattacharya, S. did her PhD with Kumar, P. .(*Corresponding author)
- 6. Tapas, S., Kumar, A., Dhindwal, S., Preeti, **Kumar, P***. Structural analysis of chorismate synthase from Plasmodium falciparum: A novel target for antimalaria drug discovery. *Int J Biol Macromol.* (2011); 49(4), 767-77.
 - Dhindwal, S. did her PhD with Kumar, P. .(*Corresponding author)
- 7. **Kumar, P***., Gómez-Gil, L., Mohammadi, M., Sylvestre, M., Eltis, L.D. & Bolin, J.T. Anaerobic crystallization and initial X-ray diffraction data of biphenyl 2,3-dioxygenase from

Burkholderiaxenovorans LB400: addition of agarose improved the quality of the crystals. *Acta Crystallogr Sect F* (2011); 67, 59-62.

Kumar, P., invented the method; Mohammadi, M., Gomez-Gil, L., Eltis, LD., Bolin J.T. & Sylvestre M. are collaborators.(*Corresponding author)

2010

- 1. Sakshi, Patil, D.N., Tomar, S., Sylvestre, M., & **Kumar**, **P***. Expression, purification, crystallization and preliminary crystallographic studies of cis-biphenyl-2,3-dihydrodiol-2,3-dehydrogenase from Pandoraea pnomenusa B-356. *Acta Crystallogr Sect F* (2010); 66:1517-20.
 - Sakshi did masters and Patil, D.N. did PhD with Kumar, P; Tomar, S. is a faculty colleague and Sylvestre, M is a collaborator. .(*Corresponding author)
- 2. Gahloth, D., Selvakumar, P., Shee, C., **Kumar, P*.**, Sharma., A.K. (Corresponding author)Cloning, sequence analysis and crystal structure determination of a miraculin-like protein from Murraya koenigii. *Arch BiochemBiophys.* (2010); 1;494(1):15-22. **Selvakumar, P. did his PhD with Kumar, P; Gahloth, D., Shee, C. did their PhD with Sharma., A.K. .(*Corresponding author)**

2009

- 1. Tomar, S., Patil, D.N., Datta, M., Tapas, S., Preeti, Chaudhary, A., Sharma, A.K., Tomar, S., **Kumar**, **P***. Crystallization and preliminary X-ray diffraction analysis of the complex of Kunitz-type tamarind trypsin inhibitor and porcine pancreatic trypsin. *Acta Crystallogr Sect F* (2009); 1;65(Pt 11):1179-81.
 - Patil, D.N., Datta, M., did their PhD and Chaudhary, A. did project with Kumar, P; Tapas, S., and Preeti did their PhD with Tomar, S.; Sharma, A.K. is a faculty colleague.(*Corresponding author)
- 2. Patil, D.N., Datta, M., Chaudhary, A., Tomar, S., Sharma, A.K. & Kumar, P*. Isolation, purification, crystallization and preliminary crystallographic studies of chitinase from tamarind (Tamarindus indica) seeds. *Acta Crystallogr Sect F* (2009); 65(Pt 4):343-5. Patil, D.N., Datta, M., did their PhD and Chaudhary, A. did project with Kumar, P; Tapas, S., and Preeti did their PhD with Tomar, S.; Sharma, A.K. is a faculty colleague. (*Corresponding author)
- 3. Patil, D.N., Preeti, Chaudhry, A., Sharma, A.K., Tomar, S., **Kumar, P***. Purification, crystallization and preliminary crystallographic studies of a Kunitz-type proteinase inhibitor from tamarind (*Tamarindus indica*) seeds. *Acta Crystallogr Sect F* (2009); 65(Pt 7):736-8. **Patil, D.N., did his PhD and Chaudhary, A. did project with Kumar, P; Preeti did her PhD with Tomar, S.; Sharma, A.K. is a faculty colleague. (*Corresponding author)**

2008

- 1. Chaudhary, N.S., Shee, C., Islam, A., Ahmad, F., Yernool, D., **Kumar, P**. & Sharma, A.K. Purification and characterization of a trypsin inhibitor from Putranjivaroxburghii seeds. *Phytochemistry*. (2008); 69(11):2120-6.
 - Kumar, P. helped in structure analysis; Chaudhary, N.S., Shee, C., did their PhD with Sharma, A.K, faculty collegue; Islam, A., Ahmad, F., Yernool, D., are collaborators.

2007

- 1. Shee, C., Singh, T.P., **Kumar, P.** & Sharma, A.K. Crystallization and preliminary X-ray diffraction studies of Murrayakoenigii trypsin inhibitor. *Acta Crystallogr Sect F* (2007); 63(Pt 4):318-9.
 - Kumar, P. did structural analysis; Shee, C. did his PhD with Sharma, A.K. Singh, T.P. is a collaborator

Post Doctoral Work

2. Horsman, G.P., Bhowmik, S., Seah, S.Y., **Kumar, P.,** Bolin, J.T. &Eltis, L.D. The tautomeric half-reaction of BphD, a C-C bond hydrolase. Kinetic and structural evidence

- supporting a key role for histidine 265 of the catalytic triad. J Biol Chem. (2007); 282(27):19894-904.
- **3.** Gomez-Gil L., **Kumar, P.,** Barriault, D., Bolin, J.T., Sylvestre, M. &Eltis, L.D. Characterization of biphenyl dioxygenase of *Pandoraea pnomenusa* B-356 as a potent polychlorinated biphenyl-degrading enzyme. *J Bacteriol*. (2007); 189(15):5705-1

4. PhD work

2004

1. Dey, S., Vijayaraghavan, R., Goel, V.K., Kumar, S., **Kumar, P**. & Singh, T.P. Design of a model peptide with a, b-dehydro-residues: Synthesis of Boc-Ile- DAla-OCH3 and its crystal structures obtained from two different solvents. *J. Mol. Struct.* (2004); 737 27-3.

2003

- 1. Vijayaraghavan, R., Makker, J., **Kumar, P.**,Dey, S., Singh, T. P. Crystal structure of Boc-Trp (CHO) ΔPhe-Ile-ΔPhe-Leu-OCH3, C48H59N6O10. *ZeitschriftfuerKristallographie New Crystal Structures* (2003); 218(1), 52-54.
- 2. Makker, J., Dey, S., **Kumar, P.**, Singh, T. P. Crystal structure of Boc-ILe-ΔPhe-Ile-OCH3, C27H43N3O7. *ZeitschriftfuerKristallographie New Crystal Structures* (2003); 218, 179-180.
- 3. Vijayaraghavan R., Makker, J., **Kumar, P.,** Dey S., Singh T.P. Design of peptides with a, b -dehydro-residues: syntheses, crystal structures and molecular conformations of two ΔPhe-Trp containing peptides. *Journal of Molecular Structure*, (2003); 654(1-3), 103-110.
- Makker, J., Dey, S., Mukherjee, S., Vijayaraghavan, R., Kumar, P., Singh, T. P. Design of peptides with a, b -dehydro-residues: synthesis, crystal structure and molecular conformation of a tetrapeptide Z-ΔVal-Val-ΔPhe-Ile-Ome. *Journal of Molecular Structure*,(2003); 654(1-3), 119-124.
- 5. Vijayaraghavan R., **Kumar, P.**, Dey S., Singh T.P. Design of peptides with branched beta-carbon dehydro- residues: syntheses, crystal structures and molecular conformations of two peptides, (I) N-Carbobenzoxy-DeltaVal-Ala-Leu-OCH3 and (II) N-Carbobenzoxy-DeltaIle-Ala-Leu-OCH3. *J. Pept. Res.* (2003); 62(2):63-9.
- 6. Mohanty A.K., Singh G., Paramasivam M., Saravanan K., Jabeen T., Sharma S., Yadav S., Kaur P., **Kumar, P**., Srinivasan A, Singh T.P Crystal structure of a novel regulatory 40-kDa mammary gland protein (MGP-40) secreted during involution. *J. Biol. Chem.*(2003); 278(16):14451-60.

<u>2002</u>

- 1. Makker, J., Dey, S., Mukherjee, S., **Kumar, P.,** Singh, T. P. Crystal structure of Boc-Leu-ΔPhe-ΔPhe-Ile-OCH3, C36H48N4O7. *Zeitschriftfuer Kristallographie-New Crystal* Structures (2002); 217(3), 372-374.
- 2. Makkar, J., Dey, S., **Kumar, P.**, Singh, T.P. Crystal structure of Boc-Leu-ΔPhe-Ile-ΔPhe-Ile-OCH3,C42H59N5O8. *Zeitschriftfuer Kristallographie New Crystal Structures* (2002); 217(3), 369-371.
- 3. **Kumar, P.**, Yadav, S. & Singh, T.P. Crystallization and structure determination of goat lactoferrin at 4.0 Å resolution: A new form of packing in lactoferrins with a high solvent in crystals. *Ind. J. Biochem. Biophys.* (2002); 39(1):16-21.

- 4. Makkar, J., Dey, S., **Kumar, P.,** Singh, T.P. Design of peptides with alpha, beta-dehydro residues: pseudo-tripeptideN-benzyloxycarbonyl-DeltaLeu-L-Ala-L-Leu-OCH3. *Acta Crystallogr C58* (2002); 212-4.
- 5. **Kumar, P.**, Khan, J.A., Yadav, S. & Singh, T.P. Crystal structure of equine apolactoferrin at 303 K providing further evidence of closed conformations of N and C lobes. *Acta Crystallogr D58* (2002); 225-32.

- 1. Singh, J.D., Milton, M.D., Bhalla, G. Khandelwal, B. L., **Kumar, P.**, Singh, T. P., Butcher, R. J. Design, synthesis and structural aspects of acyclic N3E2 (E = Se or Te) type donors and its complexes with Group 12 metals. *Phosphorus, Sulfur and Silicon and the Related Elements*. (2001); (171-172) 477-484.
- 2. Milton, M.D., Singh, J. D., Khandelwal, B. L.; **Kumar, P.**, Singh, T. P., Butcher, R. J. Design, synthesis and structural aspects of terdentate (N,O,Se/Te) donors and their competitive coordination behavior towards Pt(II). *Phosphorus,Sulfur and Silicon and the Related Elements*, (2001); (171-172) 485-492.
- 3. Tomar, S., Yadav, S., Chandra, V., **Kumar, P.**, Singh, T.P. Purification, crystallization and preliminary X-ray diffraction studies of disintegrin (schistatin) from saw-scaled viper (Echiscarinatus). *Acta Crystallogr D57*(2001);1669-70.
- 4. Vijayaraghavan, R., **Kumar, P.**, Dey, S., Singh, T.P. Design of peptides with alpha, beta-dehydro residues: a dipeptide with a branched beta-carbon dehydro residue at the (i+1) position, methyl N (benzyloxycarbonyl) alpha, beta didehydrovalyl L tryptophanate. *Acta Crystallogr C57* (2001); 1220-1.
- 5. Khan, J.A., **Kumar**, **P.**, Sharma, S., Mohanty, A.K., Jabeen, T., Paramasivam, M., Yadav, S., Srinivasan, A. & Singh, T.P. Mechanism of iron-uptake and iron-release in lactoferrins. *Proc. Ind. Nat. Sc. Acad.* B67 (2001);1-17.
- 6. **Kumar, P.,** Yadav, S., Srinivasan, A., Bhatia, K.L. & Singh, T.P. A novel 40 kDa protein from goat mammary secretions: purification, crystallization and preliminary X-ray diffraction studies. *Acta Crystallagr. D5765*; 1332-3.
- 7. Sharma, S., **Kumar**, **P**., Betzel, C., Singh, T.P. Structure and function of proteins involved in milk allergies. *J Chromatogr B Biomed Sci Appl.* (2001); 756(1-2), 183-7.
- 8. Khan, J.A., **Kumar, P.,** Paramsivam, M., Yadav, R.S., Sahni, M.S., Sharma, S., Srinivasan, A. & Singh, T.P. Structure of camel apolactoferrin at 2.6Å resolution and structural basis of its dual role as a transferrin-cum-lactoferrin. *J. Mol. Biol.* (2001); 309(3), 751-61.
- 9. Khan J.A., **Kumar, P.**, Srinivasan, A., Singh, T.P. Protein intermediate trapped by the simultaneous crystallization process. Crystal structure of an iron-saturated intermediate in the Fe3+ binding pathway of camel lactoferrin at 2.7 Å resolution. *J.Biol. Chem.* (2001); 276(39), 36817-23.
- 10. Betzel, C., Gourinath, S., **Kumar**, **P**., Kaur, P., Perbandt, M., Eschenburg, S. & Singh, T.P. Structure of a serine protease proteinase K from Tritirachium album Limber at 0.98Å resolution. *Biochemistry*. (2001); 40(10), 3080-8.

1999

1. Bhatia, S., **Kumar, P.,** Kaur, P., & Singh, T.P. Design of peptides with a ,b - dehydroresidues: synthesis, and crystal and molecular structure of a 310-helical tetrapeptideBoc-L-Val-D Phe-D Phe-L-Ile-OCH3. *J. Pept. Res.* (1999); 54, 249-256.

Other Professional activities/responsibilities

1. Teaching

Courses Taught:

B.Tech.: Structural Biology, Macromolecular Crystallography, Bioinformatics

M.Sc. : Structural Biology, Macromolecular Crystallography, Bioinformatics

Course Developed:

Macromolecular Crystallography (Institute elective), Bioinformatics: M.Sc. & B.Tech. (Biotechnology), Structural Biology: B.Tech. (Biotechnology), Structure based drug design: B.Tech. (Biotechnology), Protein Crystallography: B.Tech. (Biotechnology)

Books Edited/Authored

- 1. Biodegradation And Bioremediation of the series Env. Sci. & Engg.
- 2. Environmental Pollution: Monitoring, Modeling and Control

Research

Reviewer Assignments

Ad hoc reviewer of research papers in journal (The Journal of Biological Chemistry, ACTA D, Biochemical Journal, FEBS Journal, Journal of Structural Biology), Ph.D. and Masters Theses and research projects.

Member Research Committee

- 1. Chairman and member of SRC committees in Biotechnology, Chemistry and Chemical Engineering Departments.
- 2. Member of American Society of Microbiology, American crystallographic association, Indian crystallographic association, American Society of Microbiology

Organization of Courses/Conferences/Workshops

- 1. Co-ordinator of GIAN course on "Methods and techniques in Integrated Structural Biology: Towards structure based drug development" held from 15-21 Jan, 2018 at IIT Roorkee sponsored by MHRD.
- 1. P.I. and Convener in "Indo-US International Conference on Recent Advances in Structural Biology and drug discovery" held from 9-11 October, 2014 at Dept. of Biotechnology, IIT Roorkee.
- 2. Joint Organizing Secretary in International Conference on "Molecular Signaling :Recent Trends in Biomedical Transnatinal Research" organized by Department of Biotechnology, IIT Roorkee, JNU and NII, New Delhi and held from 17-19 December, 2014 at Department of Biotechnology, IIT Roorkee.
- 3. Co-ordinator in "Hands on Training on Modern Techniques in Biotechnology (Nao/Structural Biotechnology)" held on 07-12 January, 2013 at Centre for Continuing Education and Biotechnology Department, IIT Roorkee and sponsored by Uttarakhand State Biotechnology Department.
- 4. Co-ordinator in "Hands on Training Programme on Application of Macromolecular Crystallography Unit (MCU)" held at IIC, IIT Roorkee on October 31, 2010.

5. Co-ordinator in "Workshop for National Science Talent Scholarship" in Roorkee held in 2012 sponsored by NCERT.

Invitations

- 1. Delivered an Invited talk on "The structural basis of the enhanced pollutant degrading capabilities of engineered biophenyl dioxygenases and wild type Phthalate Dioxyenase" in 46th National Seminar on Crystallography (NSC46) held in June, 2018 and organized by IISc Bangalore. 2.Delivered an invited TEQIP lectures on Industry academia interaction held on June 2018 at DOMS, IIT Roorkee.
- 3. Delivered an invited TEQIP Lectures on Industry academia interaction held on June, 2018 at DOMS, IIT Roorkee.
- 4. Invited speaker at 42nd Annual Conference of Environmental Mutagen Society of India (EMSI) held on Jan 2018 organized by BARC-Mumbai
- 5. Delivered and invited talk on "Structural study on Rieske type Oxygenases" at International conference on microscope and 39th Annual meeting of EMSI held on July, 2018 and organized by ILS, Bhubaneswar.
- 6. Presented at Annual clinical virology symposium held in June, 2016 at Daytona beach, Florida
- 6. Delivered an invited talk on "Purification and structural characterization of an 11S globulin from Wrightia tinctoria" in 2nd Plant Proteomics Workshop organized by Department of Botany, University of Delhi at Delhi-2015
- 7. Delivered an invited talk in Indo-French symposium on the topic "Application of Structural Biology in Translational Research & Structure- Guided- Drug- Design at ACTREC-Navi Mumbai, November 19-20, 2015 on "Active-Site Plasticity is Essential to Carbapenem Hydrolysis by OXA-58 Class D-Lactamase of Acinetobacter Baumannii" organized by ACTREC Navi Mumbai.
- 8. Delivered an invited talk on "Structural studies of enzymes involved in biphenyl degrading pathway" at 42nd National Seminar on Crystallography held on Nov, 2013 and organized by JNU-Delhi
- 9. Delivered an invited talk on "Structural studies of enzymes involved in the biodegradation oftoxic aromatic compounds" at National conference on Recent Trends in Protein Structural Biology held on Dec, 2013 and organized by Jamia Millia Islamia.
- 10. Delivered an invited lecture for "Current Trends in Structural Biology (CTSB)- 2012", held during April 2012 at Department of Biophysics, AIIMS on "Biochemical studies and ligand-bound structures of biphenyl dehydrogenase from Pandoraea pnomenusa strain B-356 reveal a basis for broad specificity of the enzyme" organized by All India Institute of Medical Sciences Delhi.
- 11.Delivered an invited talk in Proteomics conference on "Structural analysis of chorismate synthase from Plasmodium falciparum: a novel target for antimalaria drug discovery" at Las Vegas, USA held in July, 2012.

Visit to outside Institute / Organization

- 1. Invited in the inauguration of Cryo-EM facility in NCBS Bangalore in Jan, 2018.
- 2. Member of the selection committee of Prime Ministers Research Fellowship (PMRF) in IIT Bombay in June, 2018
- 3. Visiting Professor at Purdue University from May-July, 2017.
- 4. ESRF-Grenoble-France for collection of Synchrotron data in Sep, 2017.
- 5. ESRF-Grenoble-France for collection of Synchrotron data in Nov, 2017.

Departmental/Institutional Responsibilities:

Departmental

- 1. O/C Macromolecular Crystallography Unit, IIC till present
- 2. O/C Bioinformatics Lab 2005-2014

Institutional

- 1. Associate Dean (Corporate Interaction, I.I.T. ROORKEE) from 2017 till present
- Chief Advisor Sports (Sports Council, I.I.T. ROORKEE) from 2013 till 2016
 Deputy Chief Advisor Students Club (I.I.T. ROORKEE) from 2010 till 2013