

## **Pinak Chakrabarti**

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**Date of Birth:** January 1, 1955  
**Place of Birth:** Gauhati, Assam, India  
**Sex:** Male  
**Nationality:** Indian

### **EDUCATIONAL QUALIFICATIONS**

1981 Ph.D., X-ray Crystallography, Indian Institute of Science, Bangalore  
1976 M.Sc., Organic Chemistry, I.I.T., Kharagpur (1st class with 1st rank)  
1974 B.Sc., Chemistry, Physics, Mathematics, Gauhati University (1st class with 1st rank)

### **PROFESSIONAL EXPERIENCE**

1997- Senior Professor (since 22-12-05, Prof. since 2003), Bose Institute, Kolkata.  
1990-97 Senior Scientist, In-charge of the X-ray Diffractometer Facility, National Chemical Laboratory, Pune.  
1989-90 Research Fellow, California Institute of Technology, Pasadena.  
1984-89 Research Associate, Professor D.C. Rees, University of California, Los Angeles. Worked on the structure of iron protein involved in nitrogen fixation.  
1982-84 Post doctoral Fellow, Professor M.G. Rossmann, Purdue University. Worked on the structure of lactate dehydrogenase from a thermophilic bacteria.  
1981-82 Post doctoral Fellow, Professor J.D. Dunitz, Swiss Federal Institute of Technology. Worked on electron density calculation using low-temperature X-ray data and structural analyses using the Cambridge Crystallographic Data Base.  
1976-80 Graduate Student, Professor K. Venkatesan, Indian Institute of Science. Worked on small molecule crystallography.

### **HONOURS AND AWARDS**

Distinguished Alumnus Award, IIT Kharagpur, 2012  
Fellow, TWAS (The World Academy of Sciences for the advancement of science in developing countries)  
The Bires Chandra Guha Memorial Lecture, INSA (2011)  
Fellow, West Bengal Academy of Science and Technology  
JC Bose National Fellow (2007-)

Fellow, Indian National Science Academy  
Fellow, Indian Academy of Sciences  
Fellow, The National Academy of Sciences  
Member, Guha Research Conference  
Member, Chemical Research Society of India  
P.S. Sarma Memorial Award for contributions in the field of Biochemistry and Allied Sciences, by the Society of Biological Chemists (2004)  
Prof. Y.T. Thathachari Prestigious Award for Science 2005 (<http://www.bhramara.org/>)  
Guha Research Medal for the best thesis (1981-82) in the Dept of Organic Chemistry, IISc  
Ajit Memorial Lecture, Indian Association for the Cultivation of Science (1994)

### **ADMINISTRATIVE RESPONSIBILITIES**

Chairman, Department of Biochemistry, Bose Institute (July 2004 – July 2006, July 2010 – July 2012; May 2014-present)  
Scientist-in-Charge, Bioinformatics Centre, Bose Institute (1998-2002, 2004-present)

### **OTHER PROFESSIONAL ACTIVITIES**

- President, Asian Crystallographic Association (2013-2016).
- Member, UG/PG Board of Studies, Department of Biotechnology, Pondicherry University (2014- ); Department of Biological Sciences, Presidency University, Kolkata (2015-19).
- Member, Advisory Committee, NIPER-Kolkata (2013-2016).
- Member of the Faculty, NIBMG Fellow and YBA Selection Committee of National Institute of Biomedical Genomics (2013-2016).
- Member, Advisory Board of Journal of Molecular Recognition (2013-)
- Member, Scientific Advisory Committee, National Centre for Cell Sciences (2011-2013).
- Vice President, Asian Crystallographic Association (2010-2013)
- Chairman, National Committee of the International Union of Crystallography (2008-2011).
- Member, National Assessment and Accreditation Council (an autonomous institution of the University Grants Commission) (2009-10).
- Member, Task Force on Bioinformatics, Department of Biotechnology (Govt of India) (2004-2013).
- Member, The Wellcome Trust-DBT India Alliance's Senior and Intermediate Fellowships Selection Committee (2009-2012).
- Member, Department of Science and Technology (Govt of India) Programme Advisory Committee in Organic Chemistry (2000-2003, 2007-2012).
- Member, Indian Crystallographic Association.
- Member, Society of Biological Chemists (India)
- Member, The Chemical Research Society of India
- Member, Indian Biophysical Society
- Organizer/chairman/speaker of various national and international symposia held in different cities in India.

- Scientific Consultant, SilicoGene Informatics Pvt. Ltd, a Chatterjee Group Company (2003).

## INTERNATIONAL ACTIVITIES

- Projects with Prof. J. Janin, CNRS, Gif-sur-Yvette (2000-2003), and with Prof. Charles Robert, Institut de Biologie et Biophysique Moléculaire et Cellulaire, CNRS UMR 8619, Bât. 430, Université Paris-Sud 11, 91405, Orsay (2009-2012), both supported by the Indo-French Centre for the Promotion of Advanced Research.
- Visiting Professor, Université Paris-Sud, Orsay (May-June, 2000; May-June, 2003, July-August, 2006).
- Nodal representative (from India) for the International Network of Protein Engineering Centres (INPEC).
- Member, International Program Committees of AsCA2009, Beijing and AsCA2010, Busan.
- Member, International Program Committees of IUCr 2014, Montreal.
- Member, International Program Committees of IUCr 2017, Hyderabad.

## RESEARCH INTEREST

Understanding the structure and folding of proteins and their interactions with other molecules, large and small, using biophysical techniques (especially, X-ray crystallography) and database analysis. Some specific topics are:

- Identification of stabilizing interactions (like CH- $\pi$ , CH-O, electrophile-nucleophile, aromatic-aromatic etc.) and their implications in protein structures and function
- Analysis of protein conformation
- Protein folding, threading and prediction of structures
- Molecular modelling and dynamics
- Molecular recognition, protein-protein complexation and ion-binding by proteins
- Biophysical studies on proteins from phage lambda and *Vibrio cholerae*
- Molecular design and docking
- Bioinformatics and proteomics
- Crystal packing and supramolecular assembly
- Biological properties of ZnO nanoparticles and their interaction of with proteins

## LIST OF PUBLICATIONS

1. Chakravarty D, Robert CH Janin J and Chakrabarti P. Changes in protein structure at the interface due to complex formation. *IUCr J* (in press).
2. Chatterjee T, Mukherjee D, Banerjee M, Chatterjee BK and Chakrabarti P (2015). Crystal structure and activity of protein L-isoaspartyl-O-methyltransferase from *Vibrio cholerae*, and the effect of AdoHcy binding. *Arch. Biochem. Biophys.* 583, 140-149.
3. Dhar J and Chakrabarti P (2015). Defining the loop structures in proteins based on composite  $\beta$ -turn mimics. *Protein Engng, Design & Selection*, 28, 153-161.
4. Chakravarty D, Chakraborti S and Chakrabarti P (2015). Flexibility in the N-terminal actin-binding domain: Clues from *in silico* mutations and molecular dynamics. *Proteins*, 83, 696-710.

5. Dhar G, Chakravarty D, Hazra J, Dhar J, Poddar A, Pal M, Chakrabarti P, Surolia A and Bhattacharyya B (2015). Actin-curcumin interaction: Insights into the mechanism of actin polymerization inhibition. *Biochemistry*, 54, 1132-1143.
6. Biswas S and Chakrabarti P (2015). Analysis of interactions and dissection of interfaces involved in RNA-protein recognition. *Protein & Peptide Letters* (in press).
7. Mukherjee D, Pal A, Chakravarty D and Chakrabarti P. Identification of the target DNA sequence and characterization of DNA binding features of HlyU, and suggestion of a redox switch for *hlyA* expression in the human pathogen *Vibrio cholerae* from *in silico* studies (2015). *Nucleic Acids Res.* 43, 1407-1417.
8. Chatterjee T, Chatterjee BK, Majumdar D and Chakrabarti P. Antibacterial effect of silver nanoparticles and the modeling of bacterial growth kinetics using a modified Gompertz model (2015). *Biochim. Biophys. Acta*, 1850, 299-306.
9. Dhar J, Chakrabarti P, Saini H, Raghava GPS, Kishore R.  $\omega$ -Turn: a novel  $\beta$ -turn mimic in globular proteins stabilized by main-chain to side-chain C-H $\cdots$ O interaction (2015). *Proteins*, 83, 203-214.
10. Mukherjee D, Datta AB and Chakrabarti P (2014). Crystal structure of HlyU, the hemolysin gene transcription activator, from *Vibrio cholerae* N16961 and functional implications. *Biochim. Biophys. Acta* 1844, 2346-2354.
11. Chakraborti S, Mandal AK, Sarwar S, Singh P, Chakraborty R and Chakrabarti P. Bactericidal effect of polyethyleneimine capped ZnO nanoparticles on multiple antibiotic resistant bacteria harboring genes of high-pathogenicity island (2014). *Colloids and Surfaces B: Biointerfaces*, 121, 44-53.
12. Nishio M, Umezawa Y, Fantini J, Weiss MS, and Chakrabarti P. CH/ $\pi$  hydrogen bonds in biological macromolecules (2014). *Phys. Chem. Chem. Phys.* 16, 12648-12683.
13. Dasgupta B, Dey S and Chakrabarti P. Water and side-chain embedded  $\pi$ -turns (2014). *Biopolymers*, 101, 441-453.
14. Chakraborti S, Dhar G, Dwivedi V, Das A, Poddar A, Chakraborti G, Basu G, Chakrabarti P, Surolia A and Bhattacharyya B (2013). Stable and potent analogues derived from the modification of the dicarbonyl moiety of curcumin. *Biochemistry* 52, 7449-7460.
15. Chakraborti S, Sarwar S and Chakrabarti P. The effect of the binding of ZnO nanoparticle on the structure and stability of  $\alpha$ -lactalbumin: a comparative study (2013). *J. Phys. Chem. B* 117, 13397-13408.
16. Chakravarty D, Guharoy M, Robert CH, Chakrabarti P and Janin J (2013). Reassessing buried surface areas in protein-protein complexes. *Protein Sci.* 22, 1453-1457.
17. Chakraborti S, Bhattacharya S, Chowdhury R and Chakrabarti P (2013). The molecular basis of inactivation of metronidazole-resistant *Helicobacter pylori* using polyethyleneimine functionalized zinc oxide nanoparticles. *PLoS ONE*, 8(8): e70776.
18. Chatterjee T, Pal A, Chakravarty D, Dey S, Saha RP and Chakrabarti P (2013). Protein L-isoaspartyl-O-methyltransferase of *Vibrio cholerae*: Interaction with cofactors and effect of osmolytes on unfolding. *Biochimie*, 95, 912-921.
19. Chakraborti S, Chakravarty D, Gupta S, Chatterjee, BP, Dhar G, Poddar A, Panda D, Chakrabarti P, Dastidar SG, Bhattacharyya B (2012). Discrimination of ligands with different flexibilities resulting from the plasticity of the binding site in tubulin. *Biochemistry*, 51, 7138-7148.
20. Chakraborti S, Joshi P, Chakravarty D, Shanker V, Ansari ZA, Singh SP and Chakrabarti P (2012). Interaction of polyethyleneimine functionalized ZnO nanoparticles with bovine serum albumin. *Langmuir*, 28, 11142-11152.

21. Dey S, Pal A, Guharoy M, Sonavane S and Chakrabarti P (2012). Characterization and prediction of the binding site in DNA-binding proteins: improvement of accuracy by combining residue composition, evolutionary conservation and structural parameters. *Nucleic Acids Res.* 40, 7150-7161.
22. Chatterjee T, Pal A, Dey S, Chatterjee BK and Chakrabarti P (2012). Interaction of virstatin with human serum albumin: spectroscopic analysis and molecular modeling. *PLoS ONE*, 7(5): e37468.
23. Joshi P, Chakraborti S, Chakrabarti P, Sing SP, Ansari ZA, Husain M and Shanker V (2012). ZnO nanoparticles as an antibacterial agent against *E.coli*. *Sci. Adv. Mater.* 4(1), 173-178.
24. Joshi P, Chakraborti S, Ramirez-Vick JE, Ansari ZA, Shanker V, Chakrabarti P and Singh SP (2012). The anticancer activity of chloroquine-gold nanoparticles against MCF-7 breast cancer cells. *Colloids Surfaces B: Biointerfaces*, 95, 195-200.
25. Mazumder A, Bandyopadhyay S, Dhar A, Lewis DEA, Deb S, Dey S, Chakrabarti P and Roy S (2012). A genetic network that balances two outcomes utilizes asymmetric recognition of operator sites. *Biophys. J.* 102, 1580-1589.
26. Ganguly HK, Majumder B, Chattopadhyay S, Chakrabarti P and Basu G (2012). Direct evidence for CH $\cdots\pi$  interaction mediated stabilization of Pro-*cis*Pro bond in peptides with Pro-Pro-Aromatic motifs. *J. Amer. Chem. Soc.* 134, 4661-4669.
27. Dey S, Chakrabarti P and Janin J (2011). A survey of hemoglobin quaternary structures. *Proteins*, 79, 2861-2870.
28. Chakraborti S, Das L, Kapoor N, Das A, Dwivedi V, Poddar A, Chakraborti G, Janik M, Basu G, Panda D, Chakrabarti P, Surolia A and Bhattacharyya B (2011). Curcumin recognizes a unique binding site of tubulin. *J. Med. Chem.* 54, 6183-6196.
29. Kumar A, Chakraborti S, Joshi P, Chakrabarti P and Chakraborty R (2011). A multiple antibiotic and serum resistant oligotrophic strain, *Klebsiella pneumoniae* MB45 having novel dfrA30, is sensitive to ZnO QDs. *Ann Clin Microbiol Antimicrob* 10:19.
30. Chakraborty S, Joshi P, Shanker V, Ansari ZA, Singh SP and Chakrabarti P (2011). Contrasting effect of gold nanoparticles and nanorods on the structure and activity of bovine serum albumin. *Langmuir*, 27, 7722-7731.
31. Chatterjee T, Mukherjee D, Dey S, Pal A, Hoque KM and Chakrabarti P (2011). Accessory cholera enterotoxin, Ace, from *Vibrio cholerae*: Structure, unfolding, and virstatin binding. *Biochemistry* 50, 2962-2972.
32. Guharoy M, Pal A, Dasgupta M and Chakrabarti P (2011). PRICE (PRotein Interface Conservation and Energetics): a server for the analysis of protein-protein interfaces. *J. Struct. Func. Genom.* 12, 33-41.
33. Joshi P, Chakraborty S, Dey S, Shanker V, Ansari ZA, Singh SP and Chakrabarti P (2011). Binding of chloroquine-conjugated gold nanoparticles with bovine serum albumin. *J. Colloid Interface Sci.* 355, 402-409.
34. Sonavane S and Chakrabarti P (2010). Prediction of active site cleft using support vector machines. *J. Chem. Inform. Modeling*, 50, 2266-2273.
35. Chatterjee T, Chakraborti S, Joshi P, Singh SP, Gupta V and Chakrabarti P (2010). The effect of zinc oxide nanoparticles on the structure of the periplasmic domain of the *Vibrio cholerae* ToxR protein. *FEBS J.* 277, 4184-4194.
36. Debnath A, Saha A, Gomes A, Biswas S, Chakrabarti P, Giri B, Biswas AK, Das Gupta S and Gomes A (2010). A lethal cardiotoxic-cytotoxic protein from the Indian monocellate cobra (*Naja kaouthia*) venom. *Toxicon* 56, 569-579.
37. Guharoy M and Chakrabarti P (2010). Conserved residue clusters at protein-protein interfaces and their use in binding site identification. *BMC Bioinformatics* 11: 286.

38. Dey S, Pal A, Chakrabarti P and Janin J (2010). The subunit interfaces of weakly associated homodimeric proteins. *J. Mol. Biol.* 398, 146-160.
39. Chakraborti S, Chatterjee T, Joshi P, Poddar A, Bhattacharyya B, Singh SP, Gupta V and Chakrabarti P (2010). Structure and activity of lysozyme on binding to ZnO nanoparticles. *Langmuir*, 26(5), 3506-3513.
40. Bahadur RP and Chakrabarti P (2009). Discriminating the native structure from decoys using scoring functions based on the residue packing in globular proteins. *BMC Struct. Biol.* 9: 76.
41. Guharoy M and Chakrabarti P (2009). Empirical estimation of the energetic contribution of individual interface residues in structures of protein-protein complexes. *J. Comput. Aided Mol. Des.* 23, 645-654.
42. Mukherjee D, Saha RP and Chakrabarti P (2009). Structural and unfolding features of HlyT, a tetrameric LysR type transcription regulator of *Vibrio cholerae*. *Biochim. Biophys. Acta*, 1794, 1134-1141.
43. Sonavane S and Chakrabarti P (2009). Cavities in protein-DNA and protein-RNA interfaces. *Nucleic Acids Res.* 37, 4613-4620.
44. Joshi P, Chakraborti S, Chakrabarti P, Haranath D, Shanker V, Ansari ZA, Singh SP and Gupta V (2009). Role of surface adsorbed anionic species in antibacterial activity of ZnO quantum dots against *Escherichia coli*. *J. Nanosci. Nanotechnol.* 9, 6427-6433.
45. Pal A, Bahadur RP, Ray PS and Chakrabarti P (2009). Accessibility and partner number of protein residues, their relationship and a webserver, ContPlot for their display. *BMC Bioinformatics* 10: 103.
46. Pal A, Bhattacharyya R, Dasgupta M, Mandal S and Chakrabarti P (2009). IntGeom: a server for the calculation of the interaction geometry between planar groups in proteins. *J. Proteomics & Bioinformatics* 2(1), 60-63.
47. Biswas S, Guharoy M and Chakrabarti P (2009). Dissection, residue conservation, and structural classification of protein-DNA interfaces. *Proteins* 74(3), 643-654.
48. Sonavane S and Chakrabarti P (2008). Cavities and atomic packing in protein structures and interfaces. *PLoS Comput. Biol.* 4(9): e1000188.
49. Dasgupta B and Chakrabarti P (2008). pi-Turns: types, systematics and the context of their occurrence in protein structures. *BMC Struct. Biol.* 8: 39.
50. Biswas S, Guharoy M and Chakrabarti P (2008). Structural segments and residue propensities in protein-RNA interfaces: comparison with protein-protein and protein-DNA complexes. *Bioinformation* 2(10), 422-427.
51. Janin J, Bahadur RP and Chakrabarti P (2008). Protein-protein interaction and quaternary structure. *Q. Rev. Biophys.* 41 (2) 133-180.
52. Chatterjee T, Saha RP and Chakrabarti P (2007). Structural studies on *Vibrio cholerae* ToxR periplasmic and cytoplasmic domains. *Biochim. Biophys. Acta* 1774, 1331-1338.
53. Dasgupta B, Chakrabarti P and Basu G (2007). Enhanced stability of *cis* Pro-Pro peptide bond in Pro-Pro-Phe sequence motif. *FEBS Letters*, 581, 4529-4532.
54. Guharoy M and Chakrabarti P (2007). Secondary structure based analysis and classification of biological interfaces: identification of binding motifs in protein-protein interactions. *Bioinformatics*, 23, 1909-1918.
55. Chakrabarti P and Bhattacharyya R (2007). Geometry of nonbonded interactions involving planar groups in proteins. *Prog. Biophys. Mol. Biol.* 95, 83-137.
56. The NMITLI-BioSuite Team (Vidyasagar et al.) (2007). BioSuite: a comprehensive bioinformatics software package (A unique industry-academia collaboration). *Curr. Sci.* 92, 29-38.

57. Janin J, Rodier F, Chakrabarti P and Bahadur R (2007). Macromolecular recognition in the Protein Data Bank. *Acta Crystallogr.* D63, 1-8.
58. Pal A, Chakrabarti P, Bahadur R, Rodier F and Janin J (2007). Peptide segments in protein-protein interfaces. *J. Biosci.* 32, 101-111.
59. Saha RP, Bhattacharyya R and Chakrabarti P (2007). Interaction geometry involving planar groups in protein-protein interfaces. *Proteins*, 67, 84-97.
60. Molecular modeling and characterization of *Vibrio cholerae* transcription regulator HlyU (2006). R.P. Saha and P. Chakrabarti. *BMC Struct. Biol.* 6, 24.
61. Saha RP, Bahadur R, Pal A, Mandal S and Chakrabarti P (2006). ProFace: a server for the analysis of the physicochemical features of protein-protein interfaces. *BMC Struct. Biol.* 6, 11.
62. Raichaudhuri A, Bhattacharyya R, Chaudhuri S, Chakrabarti P and DasGupta M (2006). Domain analysis of a groundnut calcium-dependent protein kinase: nuclear localization sequence in the junction domain is coupled with nonconsensus calcium binding domains. *J. Biol. Chem.* 281, 10399-10409.
63. Saha RP, Basu G and Chakrabarti P (2006). Cloning, expression, purification, and characterization of *Vibrio cholerae* transcriptional activator, HlyU. *Protein Expression and Purification*, 48, 118-125.
64. Saha RP and Chakrabarti P (2006). Parity in the number of atoms in residue composition in proteins and contact preferences. *Curr. Sci.* 90, 558-561.
65. Singha S, Lahiri T, Dasgupta AK and Chakrabarti P. Structural classification of protein using surface roughness index. *Online Journal of Bioinformatics*, 7(2), 74-84 (2006).
66. Guharoy M and Chakrabarti P (2005). Conservation and relative importance of residues across protein-protein interfaces. *Proc. Natl. Acad. Sci. USA*, 102, 15447-15452.
67. Datta AB, Panjekar S, Weiss MS, Chakrabarti P and Parrack P (2005). Structure of  $\lambda$  CII: implications for recognition of direct-repeat DNA by an unusual tetrameric organization. *Proc. Natl. Acad. Sci. USA*, 102, 11242-11247.
68. Saha RP, Bahadur RP and Chakrabarti P (2005). Inter-residue contacts in proteins and protein-protein interfaces and their use in characterizing the homodimeric interface. *J. Proteome Res.* 4, 1600-1609.
69. Rodier F, Bahadur RP, Chakrabarti P and Janin J (2005). Hydration of protein-protein interfaces. *Proteins*, 60, 36-45.
70. Pal L, Dasgupta B and Chakrabarti P (2005).  $3_{10}$ -helix adjoining  $\alpha$ -helix and  $\beta$ -strand: sequence, structural features and their conservation. *Biopolymers*, 78, 147-162.
71. Bhattacharyya R, Pal D and Chakrabarti, P (2004). Disulfide bonds, their stereospecific environment and conservation in protein structures. *Protein Eng. Design Selection*, 17, 795-808.
72. Bahadur RP, Chakrabarti P, Rodier F and Janin J (2004). A dissection of specific and non-specific protein-protein interfaces. *J. Mol. Biol.* 336, 943-955.
73. Dasgupta B, Pal L, Basu G and Chakrabarti P (2004). Expanded turn conformations: characterization and sequence-structure correspondence in  $\alpha$ -turns with implications in helix folding. *Proteins*, 55, 305-315.
74. Bhattacharyya R and Chakrabarti P (2003). Stereospecific interactions of proline residues in protein structures and complexes. *J. Mol. Biol.* 331, 925-940.
75. Bahadur RP, Chakrabarti P, Rodier F and Janin J (2003). Dissecting subunit interfaces in homodimeric proteins. *Proteins*, 53, 708-719.
76. Bhattacharyya R, Saha, R, Samanta, U and Chakrabarti P (2003). Geometry of interaction of histidine ring with other planar and basic residues. *J. Proteome Res.* 2, 255-263.

77. Pal L, Chakrabarti P and Basu G (2003). Sequence and structure patterns in proteins from an analysis of the shortest helices: implications for helix nucleation. *J. Mol. Biol.* 326, 273-291.
78. Chakrabarti P and Janin J (2002). Dissecting protein-protein recognition sites. *Proteins*, 47, 334-343.
79. Bhattacharyya B, Pal D and Chakrabarti P (2002). Secondary structures at polypeptide chain-termini and their features. *Acta Crystallogr.* D56, 1793-1802.
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81. Pal L, Basu G and Chakrabarti P (2002). Variants of  $3_{10}$ -helices in proteins. *Proteins*, 48, 571-579.
82. Praveen T, Das T, Sureshan KM, Shashidhar MS, Samanta U, Pal D and Chakrabarti P (2002). Silver(I) oxide – silver halide mediated alcoholysis of *O*-benzoyl-*myo*-inositol 1,3,5-orthoformates: intramolecular assistance by the sulfonyl group. *J.C.S., Perkin Trans.* 2, 358-365.
83. Pal D and Chakrabarti P (2002). On residues in the disallowed region of the Ramachandran map. *Biopolymers*, 63, 195-206.
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85. Datta AB, Chakrabarti P, Subramanya HS and Parrack P (2001). Purification and crystallization of CII: an unstable transcription activator from phage  $\lambda$ . *Biochem. Biophys. Res. Commun.* 288, 997-1000.
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88. Chakrabarti P and Pal D (2001). The interrelationships of side-chain and main-chain conformations in proteins. *Prog. Biophys. Mol. Biol.* 76, 1-102.
89. Samanta U and Chakrabarti P (2001). Assessing the role of tryptophan residues in the binding site. *Protein Engng.* 14, 7-15.
90. Pal D and Chakrabarti P (2000). Conformational similarity indices between different residues in proteins and  $\alpha$ -helix propensities. *J. Biomol. Struct. Dyn.* 18, 273-280.
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92. Hazra BG, Basu S, Pore VS, Joshi PL, Pal D and Chakrabarti P (2000). Synthesis of 11 $\beta$ -(4-dimethylaminophenyl)-17 $\beta$ -hydroxy-17 $\alpha$ -(3-methyl-1-butynyl)-4,9-estradien-3-one and 11 $\beta$ -(4-acetophenyl)-17 $\beta$ -hydroxy-17 $\alpha$ -(3-methyl-1-butynyl)-4,9-estradien-3-one: two new analogs of mifepristone (RU-486). *Steroids*, 65, 157-162.
93. Pal D and Chakrabarti P (2000).  $\beta$ -sheet propensity and its correlation with parameters based on conformation. *Acta Crystallogr.* D56, 589-594.
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97. Maji M, Hossain M, Chatterjee M, Chattopadhyay SK, Puranik VG, Chakrabarti P and Ghosh S (1999). Synthesis, characterisation and reactivity of *trans*-[Ru(L)(PPh<sub>3</sub>)Br<sub>2</sub>]; L = 2-pyridyl-*N*-(2'-methylthiophenyl)methyleneimine. Crystal structure of *trans*-[Ru(L)(PPh<sub>3</sub>)Br<sub>2</sub>]. *Polyhedron*, 18, 3735-3739.
98. Samanta U, Chakrabarti P, Naskar JP, Haiti S and Datta D (1999). Structure and metal binding of an 1*H*-1,5-benzodiazepine. *Ind. J. Chem.* 38A, 553-557.
99. Samanta U, Pal D and Chakrabarti P (1999). Packing of aromatic rings against tryptophan residues in proteins. *Acta Crystallogr.* D55, 1421-1427.
100. Pal D and Chakrabarti P (1999). Graphical representation of salient conformational features of residues in protein. *Protein Engng.* 12, 523-526.
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### Popular or Newsletter article

1. Protein-protein interactions – how to know if it is intimate, fickle or having shades in between. P. Chakrabarti. Biobytes, Vol. 2, November, 2007 (Open access newsletter, <http://biobytes.bicmku.in/bbv2proteininteraction.html>).

### PATENTS

- 1) Indian patent (Application no. 1032/KOL/2012, Publication date 08.02.2013), “A novel surface-functionalized ZnO-nanoparticles exhibiting therapeutic properties, and process for preparing the same,” Chakraborti S, Joshi P, Das T, Chakrabarti P, Chakraborty R and Mandal AK.
- 2) “Peptide antagonists for inhibiting Heat Shock Protein (Hsp16.3) of Mycobacterium tuberculosis” SUJOY K. DAS GUPTA, ABHIK SAHA, ARCHNA PATHAK SHARMA, SIDDHARTHA ROY, BHABATARAK BHATTACHARYA,

PINAKPANI CHAKRABARTI. **Applicaton #:** 20070037211 **Class:** 435007100  
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