BIOGRAPHICAL INFORMATION

1. **Name** : **CHAITALI MUKHOPADHYAY**

2. **Date of Birth** : 20th July 1960

3. **Position:** Professor

4. **Address:** Department of Chemistry
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3. **Academic Qualifications** (B. Sc. onwards):

YEAR	DEGREE	UNIVERSITY/INSTITUTION
1982	B.Sc.(Chemistry Hons.)	Presidency College, Calcutta University
1984	M. Sc (Chemistry)	Calcutta University
1990	Ph.D.	Molecular Biophysics Unit, Indian Institute of Science, Bangalore.

4. **POSITIONS HELD**

YEAR	UNIVERSITY/INSTITUTION	POSITION HELD
Jun 1990 -Jan 1993	Department of Chemistry & Biochemistry. University of Maryland, Baltimore County, Maryland, USA.	**Research Associate**
March 1993 - August 1997	Distributed Information Centre, DBT-Funded Center, Bose Institute, Kolkata.	**Information Scientist**
Sept 1997 ï August 2005	Department of Chemistry**,** University of Calcutta	**Lecturer**
Sept 2005 ï Dec 2009	Department of Chemistry**,** University of Calcutta	**Reader**
Dec 2009 - till date	Department of Chemistry**,** University of Calcutta	**Professor**
Oct 2013-Sept-2015	Department of Chemistry**,** University of Calcutta	**Head**

5. AREAS OF SPECIALISATION

Chemical and biochemical recognition, structure and dynamics of macromolecules, high resolution and two-dimensional NMR spectroscopy and other spectroscopic measurements on interacting systems, molecular modeling and molecular dynamics simulation of large systems.

6. AWARDS & MEMBERSHIP

a) State Fellowship for Merit 1976 [in Xth Standard Exam]
b) Fellowship for Merit 1982 [for B.Sc. Exam]
c) Life member of Indian Biophysical Society
d) Life member of Indian Magnetic Resonance Society
e) Elected Fellow of West Bengal Academy of Science and Technology
f) Bronze Medal from Chemical Research Society of India [2010]

7. VISITING POSITIONS:

Visiting Scientist (April 2005 - June 2005) Department of Chemistry & Biochemistry. University of Maryland, Baltimore County, Maryland, USA.

Visiting Scientist (August 2008 - January 2009) National Institute of Immunology, New Delhi.

Visiting Scientist (Nov- Dec 2015) Department of Physics, University of Illinois, Chicago, USA.

List of Publications

1. **J. Membr. Biol.** 2020, 253 (1), 11-24. Effect of Transmembrane Electric Field on GM1 Containing DMPCï Cholesterol Monolayer: A Computational Study . Z Shahzadi, C Mukhopadhyay
2. **Biochimica et Biophysica Acta (BBA)-Proteins and Proteomics**, 2020,1868 (1), 140299. Ubiquitin folds via a flip-twist-lock mechanism. M Mandal, A Das, C Mukhopadhyay
3. **Langmuir** , 2018, 34 (38), 11602-11611. Phase behavior of GM1-containing DMPCï cholesterol monolayer: experimental and theoretical study. Z Shahzadi, S Das, T Bala, C Mukhopadhyay
4. **J. Biomol. Struc. Dyn.** 2017, 35 (16), 3591-3604. Effect of glycosylation on hydration behavior at the ice-binding surface of the Ocean Pout type III antifreeze protein: a molecular dynamics simulation. S Halder, C Mukhopadhyay
5. **J. Membr. Biol.** 2017, 250 (6), 617-627. Interaction between luteinizing hormone-releasing hormone and GM1-doped cholesterol/sphingomyelin vesicles: a spectroscopic study.Z Shahzadi, C Mukhopadhyay
6. **Glycoconjugate J**.2017, 34 (2), 171-179. Localization and dynamics of the anticarcinogenic curcumin with GM_1 and other miceller assemblies. M Patra, M Mandal, A Chakrabarti, C Mukhopadhyay
7. **Carbohydrate research,** 2016, 428, 8-17Dynamics simulation of soybean agglutinin (SBA) dimer reveals the impact of glycosylation on its enhanced structural stability. S Halder, A Surolia, C Mukhopadhyay
8. **FEBS Lett., 2015,** 589, 3887-3892. Insights into the behavioral difference of water in the presence of GM1. I Basu, M. Manna, C Mukhopadhyay.

9. **RSC Advances, 2015**, 111, 91166-91176. Malachite green interacts with the membrane skeletal protein, spectrin. M. Patra, C. Mukhopadhyay, A. Chakrabarti.

10. **Phys. Chem. Chem. Phys., 2015,** 17**,** 17130-17139**.** In silico phase separation in the presence of GM1 in ternary and quaternary lipid bilayers. I Basu, C Mukhopadhyay.
11. **Glycoconjugate J., 2015,** 32, 371-384, Impact of glycosylation on Stability, Structure and Unfolding of Soybean Agglutinin (SBA): An insight from Thermal perturbation Molecular Dynamics simulations. Swagata Halder, Avadhesha Surolia and Chaitali Mukhopadhyay

12. **J. of Fluorescence, 2015,** 25(3), 707-717, Organization and Dynamics of Tryptophan Residues in Brain Spectrin: Novel Insight into Conformational Flexibility. M. Mitra et al.

13. **PloS One, 2015,** ***DOI : 10.1371*** Probing Conformational Stability and Dynamics of Erythroid and Nonerythroid Spectrin: Effects of Urea and Guanidine Hydrochloride. M. Patra, C. Mukhopadhyay, A. Chakrabarti.

14. **Food Chemistry**, 2015,176, 308-313. Peanut protein sensitivity towards trace iron: A novel mode to ebb allergic response. S. K. Ghata et al.

15. **Biochemical Roles of Eukaryotic Cell Surface Macromolecules: Advances in Experimental Medicine and Biology**. **2015, 842, 263-277**. Effect of Temperature on the Phase Behaviour of Fully Saturated DAPC Lipid Bilayer: A Comparative Molecular Dynamics Simulation Study. I Basu, C Mukhopadhyay

16. **Biophys. Biochem. Acta (Biomembranes) 2014, 1838, 328-338.** Ion channel stability of Gramicidin A in lipid bilayers: Effect of hydrophobic mismatch. Ipsita Basu, A. Chttopadhyay, Chaitali Mukhopadhyay.

17. **Phys. Chem. Chem. Phys., 2014,** 16**, 21706-21716**. Microsecond molecular dynamics simulation of guanidinium chloride induced unfolding of ubiquitin. Manoj Mandal and Chaitali Mukhopadhyay

18. ***Langmuir*****, 2014, 30 (50), pp 15244–15252.** Insights into Binding of Cholera Toxin to GM1 Containing Membrane. I Basu, C Mukhopadhyay

19. **Journal of Biomolecular Structure and Dynamics, 2014, 32, 852-865.** Binding of polarity-sensitive hydrophobic ligands to erythroid and nonerythroid spectrin: fluorescence and molecular modeling studies. Malay Patra, Madhurima Mitra, Abhijit Chakrabarti and Chaitali Mukhopadhyay.

20. **Glycoconj. J**. 2014, 31, 435-447. Capability of ganglioside GM1 in modulating interactions, structure, location and dynamics of peptides/proteins: biophysical approaches. U. L. Khatun, A. Gayen, C. Mukhopadhyay

21. **Phys. Rev. E 88, 052708 (2013)** Concentration-dependent like-charge pairing of guanidinium ions and effect of guanidinium chloride on the structure and dynamics of water from all-atom molecular dynamics simulation. Manoj Mandal and Chaitali Mukhopadhyay.

22. **PLoS ONE 8(8): e71308. doi:10.1371/journal.pone.0071308 (2013)** Binding, Conformational Transition and Dimerization of Amyloid-ϐ Peptide on GM1-Containing Ternary Membrane: Insights from Molecular Dynamics Simulation. Manna M, Mukhopadhyay C
23. **Biophysical Chemistry (2013)180-181, 66-75.** Interaction of bee venom toxin melittin with ganglioside GM1 bicelle U. L. Khatun and Chaitali Mukhopadhyay

24. **Chemistry and Physics of Lipids 170– 171 (2013) 8– 18.** Gangliosides containing different numbers of sialic acids affect the morphology and structural organization of isotropic phospholipid bicelles. U. L. Khatun, A. Gayen, Chaitali Mukhopadhyay

25. Biophysical Chemistry (2012), 168-169, 48-59. Modulation of the neurotensin solution structure in the presence of ganglioside GM1 bicelle. U. L. Khatun, S. K. Goswami, and Chaitali Mukhopadhyay

26. **Small (2012) 8, 984-990. Design and Self-Assembly of a Leucine-Enkephalin Analogue in Different Nanostructures: Application of Nanovesicles**. Pradyot Koley, Anindita Gayen, Michael G. B. Drew, Chaitali Mukhopadhyay, Animesh Pramanik.

27. **Carbohydrate Research (2012), 349, 59-72, Conformations, Dynamics and interactions of di-, tri- and pentamannoside with Mannose binding lectin: A Molecular dynamics Study** Parichita Mazumder and Chaitali Mukhopadhyay

28. **Org. Lett (2011), 13, 5512-5515 Simultaneous Parallel and Antiparallel Self-Assembly in a Triazole/Amide Macrocycle Conformationally Homologous to d-,l-α-Amino Acid Based Cyclic Peptides: NMR and Molecular Modeling Study.** Abhijit Ghorai, Anindita Gayen, Goutam Kulsi, E. Padmanaban, Aparna Laskar, Basudeb Achari, Chaitali Mukhopadhyay, and Partha Chattopadhyay

29. **Phys. Chem. Chem. Phys. (2011) DOI** 10.1039/C1CP21793C **Cholesterol driven alteration of the conformation and dynamics of phospholamban in model membranes.** Moutusi Manna & Chaitali Mukhopadhyay.

30. **Langmuir (2011) 27, 3713-3722. Molecular Dynamics Simulations of the Interactions of Kinin Peptides with an Anionic POPG Bilayer.** Moutusi Manna & Chaitali Mukhopadhyay.

31. **J. Physical Chemistry B (2011) 115, 1327-1328.** Reply to the comment on **"**Urea-Mediated Protein Denaturation: A Consensus View. Atanu Das and Chaitali Mukhopadhyay.

32. **BBA, Biomembranes (2011) 1808, 127-139**. NMR **Evidence of GM1-Induced Conformational Change of Substance P Using Isotropic Bicelles.** A. Gayen and Chaitali Mukhopadhyay

33. **Biopolymers (2010) 93, 952-967. Molecular modeling and NMR studies of benzyl substituted mannosyl trisaccharide binding to two mannose-specific lectins: Allium sativam agglutinin I and Concanavalin A.** Parichita Mazumder and Chaitali Mukhopadhyay

34. **Biopolymers (2010) 93, 845-853. LpxA : A Natural Nanotube.** Atanu Das and Chaitali Mukhopadhyay

35. **Biophysical Chemistry (2010) 147, 92-101. Structure and conformational studies on dityrosine formation in the DNA binding domain of RFX5** Madhumita Chakraborty, Dipankar Bhattacharya, Chaitali Mukhopadhyay, Abhijit Chakrabarti.

36. **Carbohydrate Research (2010) 345, 61-67. Conformational behavior of α-D-mannopyranosyl-(1→6)-α,β-D-mannose complexed with two mannose-binding plant lectins, Allium sativum agglutinin I and concanavalin A, using NMR and molecular modeling techniques.** Parichita Mazumder and Chaitali Mukhopadhyay

37. **Langmuir (2009) 25(20): 12235-42 Cause and effect of melittin induced pore formation: A computational approach.** Moutusi Manna & Chaitali Mukhopadhyay.

38. **J. Phys. Chem. B *113* (2009) 113(38):12816-24 Urea-Mediated Protein Denaturation: A Consensus View.** Atanu Das and Chaitali Mukhopadhyay.

39. **Proteins: Structure, Function and Bioinformatics (2009) 75, 1024-1034**. Mechanical Unfolding Pathway and Origin of Mechanical Stability of Proteins of Ubiquitin Family: An Investigation by Steered Molecular Dynamics Simulation. Atanu Das and Chaitali Mukhopadhyay

40. **Langmuir (2008) 24**, **10298-10305**, **Molecular Level Investigation of Organization in Ternary Lipid Bilayer: A Computational Approach**. Mondal, S. and Mukhopadhyay, C.

41. **J. Phys. Chem. B *112* (26), 7903–7908(2008), Atomistic Mechanism of Protein Denaturation by Urea.** Atanu Das and Chaitali Mukhopadhyay.

42. **Langmuir (2008) 24, 5422-5432. Evidence for Effect of GM1 on Opioid Peptide Conformation: NMR Study on Leucine Enkephalin in Ganglioside-Containing Isotropic Phospholipid Bicelles.** A. Gayen and Chaitali Mukhopadhyay

43. **Biomacromolecules (2008) 9, 974-983. GM1 Induced Partial Folding Unfolding of Native and Denatured BSA in solution.** A. Gayen, C. Chatterjee & Chaitali Mukhopadhyay.

44. **Journal of Molecular Graphics and Modeling (2008) 27, 266-274. Steered Unfolding of Ricin A and B chains.** Debabani Ganguly and Chaitali Mukhopadhyay.

45. **J. Chem. Phys. (2007) 127, 165103-165111. Application of Principal Component Analysis in Protein Unfolding: An All Atom Molecular Dynamics Simulation Study.** Atanu Das and Chaitali Mukhopadhyay.

46. **Biopolymers (2007) 86, 311-320. Extended Binding Site of Ricin B Lectin for Oligosaccharide Recognition.** Debabani Ganguly and Chaitali Mukhopadhyay

47. **Chemical Physics Letters 439 (2007) 166–170. Molecular insight of specific cholesterol interactions: A molecular dynamics simulation study.** Sumita Mondal, Chaitali Mukhopadhyay

48. **Biopolymers (2006) 83, 83-94. Binding Diversity of the Two Binding Sites of Ricin B Lectin.** Debabani Ganguly and Chaitali Mukhopadhyay

49. **J. Biomol. Struct. Dyn. (2006) 24, 269-276. Specificity of Prodan for the Self-associating Domain of Spectrin: A Molecular Docking Study.** Malyasri Bhattacharya, Chaitali Mukhopadhyay, Abhijit Chakrabarti.

50. **Spectrochim Acta A Mol. Biomol. Spectrosc. (2006) 64, 116-126. Stability and conformation of the complexes of riboflavin with aromatic hydroxy compounds in an aqueous medium.** Silpi Datta, Chaitali Mukhopadhyay, Subirnath Bhattacharya, Swapan Kumar Bose.

51. **Phys Rev E Stat Nonlin Soft Matter Phys. (2005) 72, 051928. Unfolding Dynamics of the Protein Ubiquitin: An Insight from Simulation.** Shubhra Ghosh Dastidar and Chaitali Mukhopadhyay.

52. **J Biomol Struct Dyn. (2005) 23, 183-92. Binding and Folding of Melittin in the Presence of Ganglioside GM1 Micelles.** Chiradip Chatterjee amd Chaitali Mukhopadhyay.

53. **Biopolymers (2005) 78, 197-205. Interaction and structural study of kinin peptide bradykinin and ganglioside monosialylated 1 micelle.** Chiradip Chatterjee and Chaitali Mukhopadhyay.

54. **Brit. J. of Haemat. (2005) 129, 282-286. Co-inheritance of the Hb Sun Prairie mutation with a point mutation at 5 '-UTR in the eastern Indian population.** Sarkar AA, Mukhopadhyay C, Chandra S, Banerjee S, Das MK, Dasgupta UB

55. **Spectrochim. Acta A – Mol. Biomol. Spectrosc. (2005) 62, 721-728. Studies on the riboflavin-resorcinol interaction in an aqueous medium and its pH dependence**. Datta S, Mukhopadhyay C, Bhattacharya S, S. K. Bose

56. **J. Surface Sci. Technol. (2004) 20, 237-254. Effects of Local Anesthetics on a Phospholipid Bilayer: A Comparative Molecular Simulation Study with Anesthetic Molecules of Different Strengths of Action.** Sumita Mandal, Shubhra Ghosh Dastidar and Chaitali Mukhopadhyay .

57. **Phys Rev E (2004), 70, 1. Anomalous behaviour of water around Sodium Dodecyl Micelles.** Shubhra Ghosh Dastidar and Chaitali Mukhopadhyay

58. **J. Phys. Chem. B (2004) 108, 7430-7436. Pulsed-Field Gradient and Saturation Transfer Difference NMR Study of Enkephalins in the**

Ganglioside GM1 Micelle. Chiradip Chatterjee, Barun Majumder and Chaitali Mukhopadhyay.

59. **Biochem Biophys Res Commun. (2004) 315, 866-871. Conformational alteration of bradykinin in presence of GM1 micelle.** Chiradip Chatterjee and Chaitali Mukhopadhyay.

60. **Biopolymers (2003) 70, 512-21. Structural alterations of enkephalins in the presence of GM1 ganglioside micelles.** Chiradip Chatterjee and Chaitali Mukhopadhyay.

61. **Phys Rev E (2003) 68, 021921. Structure, dynamics, and energetics of water at the surface of a small globular protein: a molecular dynamics simulation.** Shubhra Ghosh Dastidar and Chaitali Mukhopadhyay.

62. **Bull. Chem. Soc. Japan. (2003), 76, 1729. Molecular Complex Formation Between Riboflavin and Salicylate in an Aqueous Medium.** Silpi Datta, Chaitali Mukhopadhyay and Swapan Kumar Bose.

63. **Journal of Structural Chemistry (2003) 44, 790-795. Conformational Heterogeneity of a Tripeptide in the Solid State and in Solution: Characterization of a g-Turn Containing Incipient Hairpin in Solution.** Samir Kumar Maji, Debasish Halder, Arijit Banerjee, Chaitali Mukhopadhyay and Arindam Banerjee.

64. **Protein Eng. (2002) 15, 979-86. Binding free energy calculations of galectin-3-ligand interactions.** Tarun K. Mandal and Chaitali Mukhopadhyay.

65. **J Biomol Struct Dyn. (2002) 19, 1121-32. Molecular dynamics simulation GM1 in phospholipid bilayer.** Debjani Roy and Chaitali Mukhopadhyay.

66. **J. Biochem. (2002) 131, 427-435. Second Derivative Fluorescence Spectra of Indole Compounds.** Suprava Nayar, Amita Brahma, Chaitali Mukhopadhyay and Debasish Bhattacharyya.

67. **Biochem Biophys Res Commun (2002) 292, 579-585. Melittin - GM1 Interaction : A Model for a Side-by-Side Complex.** Chiradip Chatterjee and Chaitali Mukhopadhyay.

68. **Biopolymers (2001) 59, 11-23. Effect of glycosylation on structure and dynamics of MHC class I glycoprotein: a molecular dynamics study.** Tarun K. Mandal and Chaitali Mukhopadhyay.

69. **J. Biomol. Struct. Dyn. (2001) 18, 639-646. GD1a in phospholipid bilayer: a molecular dynamics simulation.** Debjani Roy and Chaitali Mukhopadhyay.

70. **Indian J Biochem Biophys. (2001) 38, 96-103. Molecular modelling of MHC class I carbohydrates.** Traun K. Mandal and Chaitali Mukhopadhyay.

71. **Protein Eng. (2001) 14, 565-71**. **Homology modeling of the ligand-binding domain of glucocorticoid receptor: binding site interactions with cortisol and corticosterone.** Raja Dey, P. Roychowdhury and Chaitali Mukhopadhyay.

72. **J Nat Prod. (2000) 63, 1531-1533**. **Structure and stereochemistry of nardostachysin, a new terpenoid ester constituent of the rhizomes of Nardostachys jatamansi.** A. Chatterjee, B. Basak, M. Saha, U. Dutta, C. Mukhopadhyay, J. Banerji, Y. Konda and Y. Harigaya.

73. **Monatschefte fur Chemie / Chemical Monthly (2000) 131, 901. 1,3-dipolar cycloadditions: Part VI – structure and conformation of cycloadducts from reactions of C-aryl-N-phenylnitrones with substituted cinnamic acid amides.** Banerji A., Maiti K.K., Halder (nee Dutta)S., Chaitali Mukhopadhyay, Banerji J., Prange T. & Neuman, A.

74. **Biochem Biophys Res Commun. (1999) 256, 6-12. Molecular modeling and experimental approaches toward designing a minimalist protein having Fc-binding activity of Staphylococcal protein A.** Sengupta J, Sinha P, Mukhopadhyay C, Ray PK.

75. **Biopolymers. 1998, 45(3): 177-90. Molecular dynamics simulation of glycoprotein-glycans of immunoglobulin G and immunoglobulin M.** Mukhopadhyay C.

76. **J Biomol Struct Dyn. (1998) 15(5):999-1008. Molecular dynamics simulation of colchicinoids.** Bothra AK, Roy S, Bhattacharyya B, Mukhopadhyay C.

77. **J Biomol Struct Dyn. (1998), 15(4):663-72**. **Modeling of Entamoeba histolytica ferredoxin**. Mukhopadhyay C, Lohia A.

78. **J Biomol Struct Dyn. (1998);15(5):959-66. A fluorescence spectroscopic and molecular dynamics study of bis-ANS/protein interaction.** Bothra A, Bhattacharyya A, Mukhopadhyay C, Bhattacharyya K, Roy S.

79. J. Biomol. Struct. Dyn. (1997) 15, 19 - 25. Role of Zinc in t-RNA acceptor stem binding by Glutamyl t-RNA Synthetase : A Molecular Modeling Study. A. Bothra, S. Roy, C. Mandal & C. Mukhopadhyay

80. **Biopolymers (1994) 34, 11 - 20. Molecular Dynamics Simulation of N-Acetyl Neuraminic Acid Containing Oligosaccharides**. C. Mukhopadhyay & C.A. Bush
81. **Biopolymers (1994) 34, 21 - 29.Conformation of Oligosaccharide Receptor for E-Selectin.** C. Mukhopadhyay, K.E. Miller & C.A. Bush

82. **Biophysical Journal (1993) 64 Issue: 2: A371-A371 Conformation And Dynamics Of Oligosaccharides Having The Lewis Core And Its (2-3) Sialylated Derivative.** Mukhopadhyay C, Miller K.E., Bush C.A.

83. **Biochemistry (1992) 31, 6703 - 6709**. **Solution Structure of Lewis-X Oligosaccharide by NMR & Molecular Dynamics Simulation**. K.E. Miller, C. Mukhopadhyay, P. Cagas & C.A. Bush

84. Biopolymers (1991) 31, 1737 – 1746. Molecular Dynamics of Lewis Blood Group & Related Oligosaccharides. C. Mukhopadhyay & C.A. Bush

85. **J. Mol. Struct. (1989) 194, 203 - 214**. **Computer Simulation of Protein-Carbohydrate Complexes : Application to L-arabinose-binding Protein and Pea Lectin**. V.S.R. Rao, M.Biswas, C. Mukhopadhyay & P.V. Balaji.

86. **Int. J. Biol. Macromol. (1989), 11, 194 - 200. Computer Modelling Approach to Study the Modes of Binding of α, β-Anomers of D-galactose, D-fucose, D-glucose to L-arabinose-binding Protein.** C. Mukhopadhyay & V.S.R. Rao

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BOOK CHAPTERS:

88. **Computer Simulation of Protein-Carbohydrate Complexes : Application to Concancavalin A & L-arabiose-binding Protein** in **Computer Modelling of Carbohdrate Molecules** - Ed. by A.D. French & J.W.Brady, **ACS Symp. Series No. 430, ACS, Wash D.C. 1990, pp 361 - 376.** V.S.R. Rao, B.V.S. Reddy, C. Mukhopadhyay & M. Biswas

89. **Recent Progress in Medicinal Plants, Volume 12 (2006) pp 403-412. Oligosaccharide Recognition by Ricin B** : Debabani Ganguly and Chaitali Mukhopadhyay Ed Anil K. Sharma et al, Stadium Press, LIC, Houston, Texas-USA.