Dr. Madhu Chopra
Assistant Professor &
Coordinator Bioinformatics Facility

Title	Dr.	First Name	Madhu	Last Name	Chopra	Photograph

Designation	**Assistant Professor**
Address	**Dr. B. R. Ambedkar Center for Biomedical Research, North Campus, University of Delhi, Delhi 110007, India**
Phone No Office	**91-11-27666272, 27667151**
Residence	**1652, Ground Floor, Outram Lines, Kingsway Camp, Delhi 110009**
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Educational Qualifications

Degree	Institution	Year
Ph.D.	**Department of Chemistry, University of Delhi**	**1995**
PG	**Department of Chemistry, University of Delhi**	**1992**
UG	**University of Delhi**	**1989**
Any other qualification	**NET QUALIFIED**	**1992**

Career Profile

1. **Dr. B. R. Ambedkar Center for Biomedical research, Assistant Professor, Since December 2009**
2. **Dr. B. R. Ambedkar Center for Biomedical research, Research Scientist, November 1997 - 2009**
3. **Dr. B. R. Ambedkar Center for Biomedical research, Research Associate (CSIR), April 96 – October 1997**

Awards & Distinctions

Drug Discovery Hackathon Phase I- Award (DDH-2020), open source drug discovery Hackathon against Covid-19, Organised by Innovation Cell, Ministry of Education also selected for Phase II project.

Administrative Assignments

1. Coordinator Bioinformatics Facility Sponsored by DBT since 2006 till date
2. Coordinator NAAC from ACBR since 2012-2018
3. Radiological Safety Officer from 2006 to 2014
4. In-Charge Library ACBR from 2007 to 2014
5. In-Charge Instrumentation facility such as LC-MS, HPLC, and Central Instrumentation facility of ACBR till April 2011
6. Coordinator/examiner/superintendent of examination for courses of Biomedical Sciences from time to time.
7. Coordinator of SUMMER UNDERGRADUATE RESEARCH TRAINING PROGRAMME 2005, 2002 & 2001

Areas of Interest / Specialization

- **Computer Aided Drug Design and Development**
- **Medicinal Chemistry**
- **Nanoparticle mediated drug delivery**

Our future plans include…..

- To continue with research projects involving modelling of various anticancer and infection targets: Pharmacophore modelling, Machine learning and AI based drug design, 3D QSAR, docking and virtual screening for development novel lead/drug molecules.
- Virtual screening of plant derived molecules, building databases for virtual screening for drug like compounds, meta-analysis of cancer genomics data.
- Development of nanoparticle-based drug delivery agents
- Initiate collaborative programmes with other institutions for enriching biodiversity information resources and promoting human resource development in drug discovery and bioinformatics.

Subjects Taught

M.Sc.

1st Semester: Advanced Organic Chemistry I
2nd Semester: Advanced Organic Chemistry II
3rd Semester: Analytical and Biomedical Techniques & Instrumentation, Molecular oncology
4th Semester: Advanced Medicinal Chemistry,
Concepts in Drug Discovery and Mechanism
Bioinformatics, computational biology and drug designing

Ph.D.

1st semester Techniques in Biomedical Sciences
2nd semester Computational biology & drug design

Research Guidance

Supervision of awarded Doctoral Thesis11

1. **Nalini Yadav**, **September 2018,** "Synthesis, characterization and biological evaluation of new 1,3,4-oxadiazole thione derivatives and sitosteryl esters as potential anticancer agents."
2. **Lubna Wasim, September 2017**"Understanding the mechanism of action of HDAC inhibitors in epigenetic regulation of cancer"
3. **Monika Sharma, 2016** "3D QSAR and virtual screening for development of novel histone deacetylase(HDAC) inhibitors.
4. **Manisha Sikka, 2016 "**Investigation of combined effect of Cyclooxegenase – 2 Inhibitor, Etoricoxib and Cholecystokinin receptor -2 (CCK-2) antagonists on pancreatic cancer cells"

5. **Monal Sharma, March, 2012**,Studying the effect of Suberoylanilide hydroxamic acid (SAHA), a HDAC inhibitor and Vitamin E on Human Cerivcal (HeLa) cancer cell line.
6. **Ruby Gupta, February 2012,** "Pharmacophore Modeling, Virtual Screening and Development of COX-2 Selective Inhibitors.
7. **Shweta Tripathi**, **March 2011**, "Mechanistic Study Involving Antiproliferative Effect of Cyclooxygenase-2 Selective Inhibitor on Human Cancer Cell Lines."
8. **Rakhi Srivastava, February 2011,**"Screening and Isolation of Active Principles from *Boerhaavia diffusa* as Potential Anticancer agents and their Mechanistic Study"
9. **Joyita Chaudhary, March 2009**: "Biological Evaluation of Quinazolinone Derivatives On Cholecystokinin-B Receptor Expressing Cell Lines."
10. **Saroj Kumari December 2006** "Synthesis and evaluation of cholecystokinin receptor specific antagonists taking lead from naturally occurring ligand.
11. **Mita Sarkar, July 2006** "Studies on Oxidative stress and antioxidants in thyroid dysfunction"

Supervision of Doctoral Thesis, under progress = 5

12. **Priya Poonia, 2016-** Design and development of subtype selective HDAC inhibitors as anticancer agents.
13. **Sumeet Baweja, 2016 -** To understand molecular mechanism of HDAC inhibition with subtype selective inhibitors.
14. **Prakash Jha, 2017**- Design and Development of novel PAD2 inhibitors aspotential therapeutics for breast cancer treatment
15. **Vineeta Teotia**, **2018**- Design and development of target specific anticancercompounds
16. **Prerna Rajoria, 2021-** Target based design and development of molecules against human diseases.

Other Research scholars worked in collaboration = 3

17. **Gautam Behl, (SRF, ICMR**) Development of nanoparticle-based drug delivery agents. (Completed Ph.D. 2013)
18. **Priyanka Verma**, Joint Registration at AIIMS with Dr. Krishana Dalal, "Estimation of the level of Cartilage Oligomeric Matrix protein and Designing of an Inhibitor" (Completed Ph.D. 2013)
19. **Praveen Kumar,** Design and Development of HDAC inhibitors as anticancer compounds. (Ph.D. Completed, 2017)

Supervision of awarded M.Sc. dissertations= 55

1. **Purvashi Pasrija**, 2021: A review on Artificial Intelligence in drug design and discovery.
2. **Mandavi Raji Sarraf**, 2021: Modern drug discovery approaches for development of Anticancer Drugs

3. **Lucky, 2021:**Targeting telomerase for the treatment of cancer with different kinds of inhibitors & their role in bone marrow failure syndrome and other diseases and to elucidate the binding site of VX-222 on hTERT, pharmacophore generation and virtual screening
4. **Harshita Saini, 2021:** To study protein-protein interaction networks of various Histone Deacetylases, to categorize these interacting proteins according to their molecular and cellular function and to identify unique pathways they regulate.
5. **Mohit Kumar, 2020**: Antiproliferative effect of HDAC inhibitors and c-MET inhibitor on Gastric Cancer.
6. **Dashleen Kaur, 2020:**Investigating Cytotoxicity of HDAC6 Inhibitor in Cervical Cancer Cells (HeLa) & Evaluation of HDAC isoform selectivity in the early stages of drug discovery
7. **Manju, 2020:** Investigating Cytotoxicity of CDK Inhibitors in Cervical Cancer Cells (HeLa)
8. **Neeraj Saini**, **2019**: To elucidate the combined effect of pan HDAC inhibitor and natural flavanoid against cervical cancer (HeLa) cells.
9. **Anupam Kaushik**, **2019**: Deciphering combination therapy involving cell cycle kinases and other anticancer targets through protein-protein interaction (PPI) networks.
10. **Vagish Pande** , **2019**: Designing ligands for Intestinal Cell Kinase using homology modeling, pharmacophore based virtual screening and docking studies.
11. **Vineeta Teotia, 2018,** Investigating Cytotoxicity of HDAC6 Inhibitor Alone and In Combination with Topoisomerase Inhibitor in Cervical Cancer Cells (HeLa).
12. **Seetha Lakshmi Venu, 2018**, Combination effect of HDAC inhibitor and c-MET inhibitors on Cancerous cell line
13. **Someshwar Nath Jha, 2018**,Pharmacophore Based Virtual Screening and Docking to identify HDAC6 inhibitors using DRUGBANK Database.
14. **Yamini, 2017**, Synthesis and characterization of polymeric nanogels for the delivery of panobinostat
15. **Shafali Saini, 2017**, To study anti-cancer activity of sitosteryl esters against cervical cancer cells (HeLa)
16. **Shreya, May 2016**, In Silico studies of Phytosterols and their derivatives on Cholesterol absorption mediated by NPC1L1
17. **Sulakshana Deka, May 2016,**Anti – proliferative effect of Vorinostat and its nano-formulation on growth of HeLa cells
18. **Preety Loaura**, **May 2016**, Synthesis and Characterization of Polymeric Nanogel for the Delivery of Doxorubicin,
19. **Namit Dey**, **May2015**, "Co-delivery of etoposide and vorinostat encapsulated on biodegradable poly(oligoethylene glycol)methylacrylate PEOMA nanaogels as anticancer combinatorial drug treatment."
20. **Dounai Annajarvis**, **May 2015**, "Synthesis and evaluation of sitosteryl esters as potential anti-cancer agents."
21. **Basabi Pegu, May 2014*, "****In silico*** docking and evaluation of antiproliferative activity of plant based Sitosteryl esters as Estrogen Receptor modulators."

22. **Manisha Kadam, May 2014**, "Synergistic Effect of HDAC inhibitor and Topoisomerase inhibitors on Human cervical cancer cell lines."
23. **Neha Kanojia**, **May 2013**, "To study the antiproliferative activity of Panobinostat (PS), a Histone deacetylases (HDAC) inhibitor in combination with Curcumin on human cervical cancer cells and comparative *in silico* binding study of Panobinostat in HADAC1"
24. **Bhawani, May 2013,** "To study the anti-proliferative activity of Sitosteryl oleate,its analogs Sitosteryl acetate and Sitosteryl benzoate on human glioblastoma cell line (U87).Elucidation of a putative mechanism of action of Sitoteryl oleate in these cells.
25. **Noopur Singh**, May 2012, "Elucidating possible mechanism for antiproliferative action of sitosteryl oleate and hypothesizing suitable analogues with better activity.
26. **Utpraksha Vaish,** May 2012, "To explicate the biochemical efficiency of novel cyclooxegenase-2 inhibitor.
27. **Chhaya Dhiman**,May 2011, "Elucidating the probable mechanism of active principles from Beorhaavia diffusa.
28. **Vivek kant Mishra**, May 2011, "Synthesis and characterization of biodegradable nanoparticle for targeted drug delivery".
29. **Tahir,**May 2011, "Understanding the antiproliferative action of Etoricoxib".
30. **Nalini Yadav,** May 2010,"Screening of the chemically synthesized active principle (Sitosterol Oleate) from Boerhaavia diffusa as potential anticancer agents.
31. **Deepshikha,** May 2010, "Targeting Cancer through Cholecystokinin-B Receptor Antagonists."
32. **Astha Gupta**, *May 2009*, "Three dimensional pharmacophore modeling of histone deacetylase (HDAC) inhibitors.
33. **Poonam**, *May 2009*, "Isolation and purification of Cytotoxic Constituents from Boerhaavia diffusa root extract and to study the effect of one of the active principles on Apoptosis in U-87 cell line"
34. **Angad Garg**, May 2008 "To study the effect of COX-2 selective inhibitor on proliferation of pancreatic cell line (Mia Paca-2)"
35. **Manish Muhuri**, May 2008 "To study the expression of CCK-B/Gastrin Receptor on various cell lines and to evaluate the biological activity of quinazolinone derivatives."
36. **Paromita Gupta**, May 2008 "Synthesis of Histone Deacetylase Inhibitors and to study the effect of SAHA for inducing oxidative injury and apoptosis in Hela cell line."
37. **Garima Chauhan**, "Screening and isolation of potential cytotoxic natural compounds from the leaf extract of Boerhaavia diffusa."
38. **Sheetal Kaw**, *May 2007*, "To study the expression of CCK-BR/ CCK-CR in various cancer cell lines and to determine the antagonistic activity of new quinazolinone derivative on CCK-BR positive cell lines
39. **Anamika Ghosh,***May 2007,* "In silico designing & synthesis of novel HDAC inhibitors and

studying the synergistic effect of VPA with known anticancer compounds."

40. **Ishan Shankar**, *May 2007* "To predict the structure of DNA Gyrase subunit A and B of Neisseria gonorrhoea using the homology modelling technique."
41. **Priyanka Kant**, *May 2007* "Standardization of Analytical technique for purification of Ciprofloxacin derivatives using HPLC."
42. **Rajni Bala**, *May 2007*, "Radiolabeling and biological evaluation of 99mTc labelled cycloserine DTPA conjugate for Tuberculosis diagnosis."
43. **Amit Kumar Yadav**, *June 2006*, "Three Dimensional Pharmacophore Modeling, *In Silico* Screening and Docking Studies for Identification of Novel Leads as Cyclooxygenase-2 Selective Inhibitors"
44. **Lunminlal Kipgen**, *June 2006*, "Virtual screening for novel CCK-B antagonists using pharmacophore based database search"
45. **Rajeshwari Singh**, *July 2006,* "To study the role of non-steroidal anti-inflammatory drugs (NSAIDs) in apoptosis using HeLa Cell line.
46. **Swati Gupta**, *June 2005*, "Three Dimensional Pharmacophore Modeling ofCOX – 2 Inhibitors"
47. **Amresh Prakash**, *June 2005*, " In silico protein Structure Prediction and Pharmacophore Modeling"
48. **Pronoti Sarkar**, *June 2005*, "Isolation and Screening of Anticancer Metabolites from *Boerhaavia diffusa* and *Oxalis corniculata*
49. **Puneet Kumar Gupta**, *June 2004* Isolation and screening of anticancer metabolites from Boerhaavia diffusa (part-I) and Homology Modelling of Cholecystokinin Receptor Type A (Part II)
50. **P. V. Sunandini,** 2004, "Synthesis of CCK-B/Gastrin Receptor Specific Antagonist using Asperlicin"
51. **Anubha Singh**, *June 2003*, "Synthesis of Benzopyran Derivatives and to study the Antifertility Potential in Rats"
52. **Ram Azore***, June 2003, "T*o Check the Expression of CCK-B Receptor in Tumour Cell Lines"
53. **Asha Kumari***, June 2002* "Expression of Cholecystokinin type B Receptor Using pEG Vector and to Study Interaction of Synthesized Ligand Using Fluorescence Techniques.
54. **Nitu Kumari**, *July 2002* "Radiolabeled Nonpeptidic Ligand for Targeting Cholecystokinin – B/Gastrin Receptor Expressing Tumors & Expression of CCK-B receptor in pEG vector"
55. **Saroj Kumari,** *June 2001* "Design, Synthesis and Evaluation of non Peptidic CCK-B/gastrin Receptor Specific Antagonists Taking Lead from Naturally Occurring Ligand."

Supervision of M.Sc Summer Projects*(2 months duration)Completed 40 Projects*

Publications Profile

1. ***Books/Monographs (Authored/Edited)***

Year of Publication	**Title**	**Publisher**	**Co-Author**
2008, 2012 (2nd ed.)	**Medicinal Chemistry**	**ANE Books (CRC PRESS)**	V. K. Ahluwalia

2. ***Research papers published in Refereed/Peer Reviewed Journals = 39***

Total # citations = 695; H-index = 17; Total Impact factor = 115.961; Average IF = 2.973.

1. Jha,P., Singh, P., Arora, S., Sultan, A., Nayek, A., Ponnusamy, K., Syed, M.A., Dohare, R., Chopra, M. (2022)Integrative multi-omics and in silico analysis reveals the role of ARHGEF1 and its screened antagonist in mild and severe COVID-19 patients, J Cell Biochem Jan 17. doi: 10.1002/jcb.30213. [Wiley, **IF 4.429**]
2. Pawar, A., Jha, P., Chopra, M., Chaudhry, U., Saluja, D. (2020) Screening of natural compounds that targets glutamate racemase of *Mycobacterium tuberculosis* reveals the anti-tubercular potential of flavonoids, Scientific Reports, 10, Article no. 949, Doi: 10.1038/s41598-020-57658-8. [Nature, **IF 4.379**]
3. Sharma, M., Jha, P., Verma, P., **Chopra, M***. (2019). Combined comparative molecular field analysis, comparative molecular similarity indices analysis, molecular docking and molecular dynamics studies of histone deacetylase 6 inhibitors, *Chemical Biology and Drug Design*, 93(5): 910-925. https://doi.org/10.1111/cbdd.13488.[Wiley, **IF 2.817**].
4. Pawar A, Jha P, Konwar C, Chaudhry U, Chopra M, Saluja D. (2019). Ethambutol targets the glutamate racemase of Mycobacterium tuberculosis-an enzyme involved in peptidoglycan biosynthesis. *Appl Microbiol Biotechnol.* 103(2):843-851. doi: 10.1007/s00253-018-9518-z. [Springer, **IF-4.813**]
5. Sinha, R., Singh, P., Saini, N. K., Kumar, A., Pathak, R., Chandolia, A., **Chopra, M**.… Bose, M. (2018). Methyl-accepting chemotaxis like Rv3499c (Mce4A) protein in Mycobacterium tuberculosis H37Rv mediates cholesterol-dependent survival. *Tuberculosis*, *109, 52-60*. https://doi.org/10.1016/j.tube.2018.01.004. [Elsevier, **IF- 3.313**]
6. Wasim, L., &**Chopra, M.*** (2018). Synergistic anticancer effect of panobinostat and topoisomerase inhibitors through ROS generation and intrinsic apoptotic pathway induction in cervical cancer cells. *Cellular Oncology,41(2), 201-212* . https://doi.org/10.1007/s13402-017-0366-0. [**Springer, IF-6.730**].
7. Kumar, P., Wasim, L., **Chopra, M.***, & Chhikara, A. (2018). Co-delivery of Vorinostat and Etoposide Via Disulfide Cross-Linked Biodegradable Polymeric Nanogels: Synthesis, Characterization, Biodegradation, and Anticancer Activity. *AAPS PharmSciTech, 19(2), 634-*

647. https://doi.org/10.1208/s12249-017-0863-5. [AAPS, **IF-3.246**]

8. Kumari, S., Chowdhury, J., Sikka, M., Verma, P., Jha, P., Mishra, A. K., … **Chopra, M.*** (2017). Identification of potent cholecystokinin-B receptor antagonists: Synthesis, molecular modeling and anti-cancer activity against pancreatic cancer cells. *MedChemComm*, *8*(7), 1561-1574. https://doi.org/10.1039/ c7md00171a. [Royal Society of Chemistry, IF – **2.394**]
9. Kapoor, H., Yadav, N., **Chopra, M**., Mahapatra, S. C., & Agrawal, V. (2017). Strong anti-tumorous potential of Nardostachys jatamansi rhizome extract on glioblastoma and In Silico analysis of its molecular drug targets. *Current Cancer Drug Targets*, *17*(1), 74-88.https://doi.org/10.2174/1570163813666161019143740. [Bentham, IF-**3.428**]
10. Yadav, N., Kumar, P., Chhikara, A., &**Chopra, M.*** (2017). Development of 1,3,4-oxadiazole thione based novel anticancer agents: Design, synthesis and in-vitro studies. *Biomedicine and Pharmacotherapy*, *95, 721-730*. https://doi.org/10.1016/j.biopha.2017.08.110. [**Elsevier, IF-6.529**]
11. Kumar, P., Yadav, N., hhikara, A., **Chopra, M.*** (2017). Combinatorial Solid Phase Synthesis: Techniques, Characterization and its Application in Drug Development, *Current Biochemical Engineering*, Vol 4 (1), 9-33. DOI 10.2174/2212711903666160622085741
12. Kumar, P., Behl, G., Sikka, M., Chhikara, A., &**Chopra, M.*** (2016). Poly(ethylene glycol)-co-methacrylamide-co-acrylic acid based nanogels for delivery of doxorubicin. *Journal of Biomaterials Science, Polymer Edition*, *27*(14). https://doi.org/10.1080/09205063.2016.1207588. [**Taylor & Francis**, IF-**3.113**]
13. Verma, P., Dalal, K., &**Chopra, M**.* (2016). Pharmacophore development and screening for discovery of potential inhibitors of ADAMTS-4 for osteoarthritis therapy. *Journal of Molecular Modeling*, *22*(8). https://doi.org/10.1007/s00894-016-3035-8. **[Springer, IF-1.810**]
14. Wasim, L., &**Chopra, M.*** (2016). Panobinostat induces apoptosis via production of reactive oxygen species and synergizes with topoisomerase inhibitors in cervical cancer cells. *Biomedicine and Pharmacotherapy*, *84:*1393-1405. https://doi.org/10.1016/j.biopha.2016.10.057.

[**Elsevier, IF-6.529**]

15. Sharma, G., Kapoor, H., **Chopra, M.**, Kumar, K., & Agrawal, V. (2014). Strong larvicidal potential of Artemisia annua leaf extract against malaria (Anopheles stephensi Liston) and dengue (Aedes aegypti L.) vectors and bioassay-driven isolation of the marker compounds. *Parasitology Research*, *113*(1). https://doi.org/10.1007/s00436-013-3644-4. **[Springer, IF – 2.403]**
16. Behl, G., Sikka, M., Chhikara, A., &**Chopra, M**.* (2014). PEG-coumarin based biocompatible self-assembled fluorescent nanoaggregates synthesized via click reactions and studies of aggregation behavior. *Journal of Colloid and Interface Science*, *416*: 151-160 https://doi.org/10.1016/j.jcis.2013.10.057. [Elsevier, IF-**8.128**]
17. Behl, G., Sharma, M., Sikka, M., Dahiya, S., Chhikara, A., &**Chopra, M.*** (2012). Gallic acid loaded disulfide cross-linked biocompatible polymeric nanogels as controlled release system: Synthesis, characterization, and antioxidant activity. *Journal of Biomaterials Science, Polymer*

Edition, *24*(7). https://doi.org/10.1080/09205063.2012.723958. [Taylor & Francis, **IF-3.113**]

18. 2D-QSAR, Docking Studies, and *In Silico* ADMET Prediction of Polyphenolic Acetates as Substrates for Protein Acetyltransferase Function of Glutamine Synthetase of *Mycobacterium tuberculosis* Prija Ponnan, Shikhar Gupta, **Madhu Chopra**, Rashmi Tandon, Anil S. Baghel, Garima Gupta, Ashok K. Prasad, Ramesh C. Rastogi, Mridula Bose, and Hanumantharao G. Raj, ISRN Structural BiologyVolume **2013**, Article ID 373516, 12 pages,http://dx.doi.org/10.1155/2013/373516.
19. Kumari, S., Chowdhury, J., Mishra, A. K., Chandna, S., Saluja, D., &**Chopra, M.*** (2012). Synthesis and Evaluation of a Fluorescent Non-Peptidic Cholecystokinin-B/Gastrin Receptor Specific Antagonist for Cancer Cell Imaging. *ChemBioChem*, *13*(2). https://doi.org/10.1002/cbic.201100593.[Wiley, IF-**3.164**]
20. Patra, M. C., Kumar, K., Pasha, S., &**Chopra, M.*** (2012). Comparative modeling of human kappa opioid receptor and docking analysis with the peptide YFa. *Journal of Molecular Graphics and Modelling*, *33*. https://doi.org/10.1016/j.jmgm.2011.10.007. [Elsevier, IF- 2.518]
21. Pasricha, R., Chandolia, A., Ponnan, P., Saini, N. K., Sharma, S., **Chopra, M.**, … Bose, M. (2011). Single nucleotide polymorphism in the genes of mce1 and mce4 operons of Mycobacterium tuberculosis: Analysis of clinical isolates and standard reference strains. *BMC Microbiology*, *11*. https://doi.org/10.1186/1471-2180-11-41. [BioMedCentral, IF-3.605]
22. Behl, G., Sharma, M., Dahiya, S., Chhikara, A., &**Chopra, M.*** (2011). Synthesis, characterization, and evaluation of radical scavenging ability of ellagic acid-loaded nanogels. *Journal of Nanomaterials*, *2011*. https://doi.org/10.1155/2011/695138. [Hindawi, IF 2.986]
23. **Chopra, M.***, Srivastava, R., Saluja, D., & Dwarakanath, B. S. (2011). Inhibition of human cervical cancer cell growth by ethanolic extract of Boerhaavia diffusa Linn. (punarnava) root. *Evidence-Based Complementary and Alternative Medicine*, *2011*. https://doi.org/10.1093/ecam/nep223. [Hindawi, IF – 2.629]
24. Pandey, V., **Chopra, M.,**& Agrawal, V. (2011). In vitro isolation and characterization of biolarvicidal compounds from micropropagated plants of Spilanthes acmella. *Parasitology Research*, *108*(2). https://doi.org/10.1007/s00436-010-2056-y. [Springer, IF – 2.403]
25. Mathur, R., Suman, S., Beaume, N., Ali, M., Bhatt, A. N., **Chopra, M**., … Dwarakanath, B. S. (2010). Interaction and structural modification of topoisomerase IIα by peptidyl prolyl isomerase, pin1: An In Silico study. *Protein and Peptide Letters*, *17*(2). https://doi.org/10.2174/092986610790226030. [Bentham, IF-1.89]
26. Bansal, S., Ponnan, P., Raj, H.G. *et al.* Autoacetylation of Purified Calreticulin Transacetylase Utilizing Acetoxycoumarin as the Acetyl Group Donor. *Appl Biochem Biotechnol* **152,** 170–176 (2009). https://doi.org/10.1007/s12010-008-8394-x, [Springer, IF-2.926].
27. Dahiya, S., Chuttani, K., Khar, R. K., Saluja, D., Mishra, A. K., &**Chopra, M**.* (2009). Synthesis and evaluation of Ciprofloxacin derivatives as diagnostic tools for bacterial infection by Staphylococcus aureus. *Metallomics*, *1*(5): 409-417. https://doi.org/10.1039/b908474f. [Royal Society of Chemistry, IF- 4.526]
28. Chaudhary, S., Vats, I. D., **Chopra, M**., Biswas, P., & Pasha, S. (2009). Effect of varying chain

length between P1 and P1′ position of tripeptidomimics on activity of angiotensin-converting enzyme inhibitors. *Bioorganic and Medicinal Chemistry Letters*, *19*(15). https://doi.org/10.1016/j.bmcl.2009.05.079. {Elsevier, IF-2.823]

29. **Chopra, M**.*, Gupta, R., Gupta, S., & Saluja, D. (2008). Molecular modeling study on chemically diverse series of cyclooxygenase-2 selective inhibitors: Generation of predictive pharmacophore model using Catalyst. *Journal of Molecular Modeling*, *14*(11). https://doi.org/10.1007/s00894-008-0350-8. [Springer, IF-1.810]
30. PUBLISHED ARTICLE - Counterfeit Medicines - The Global Haza8rd**,** Saurabh Dahiya, Anil. K. Mishra, Roop. K. Khar, **Madhu Chopra** and Aruna Chhikara, Pharmainfo. net, Vol. 6 Issue 4, 2008
31. Sarkar, M., Varshney, R., **Chopra, M**., Sekhri, T., Adhikari, J. S., & Dwarakanath, B. S. (2006). Flow-cytometric analysis of reactive oxygen species in peripheral blood mononuclear cells of patients with thyroid dysfunction. *Cytometry Part B - Clinical Cytometry*, *70*(1). https://doi.org/10.1002/cyto.b.20082. [Wiley, IF – 3.058]
32. Mishra, A. K., **Chopra, M**.*, & Jain, V. (2005). Convenient route for synthesis of bifunctional chelating agent: 1-(p-aminobenzyl)ethylenediaminetetramethylphosphonic acid-folate conjugate (Am-Bz-EDTMP-folate). *Chemistry Letters*, *34*(8). https://doi.org/10.1246/cl.2005.1098. [The Chemical Society of Japan, IF – 1.361]
33. **Chopra, M.***, & Mishra, A. K. (2005). Ligand-based molecular modeling study on a chemically diverse series of cholecystokinin-B/gastrin receptor antagonists: Generation of predictive model. *Journal of Chemical Information and Modeling*, *45*(6): 1934-42. https://doi.org/10.1021/ci050257m. [American chemical Society, 4.956]
34. Kumari, S., Kalra, N., Mishra, P., Chutani, K., Mishra, A., &**Chopra, M.*** (2004). Novel 99mTc radiolabeled quinazolinone derivative [Qn-In]: Synthesis, evaluation and biodistribution studies in mice and rabbit. *Nuclear Medicine and Biology*, *31*(8). https://doi.org/10.1016/j.nucmedbio.2004.03.014. [Elsevier, IF-2.408]
35. Mishra, A. K., Panwar, P., **Chopra, M.**, Sharma, R. K., & Chatal, J.-F. (2003). Synthesis of novel bifunctional Schiff-base ligands derived from condensation of 1-(p-nitrobenzyl)ethylenediamine and 2-(p-nitrobenzyl)-3-monooxo-1,4,7-triazaheptane with salicylaldehyde. *New Journal of Chemistry*, *27*(7). https://doi.org/10.1039/b300621m. {Royal Society of Chemistry, IF-3.591]
36. Ahluwalia, V. K., **Chopra, M**.*, & Chandra, R. (2000). A convenient synthesis of novel pyrimidine analogues of o-hydroxy chalcones an pyrano [2,3-d]pyrimidines and their biological activities. *Journal of Chemical Research - Part S*, (4). [IF-0.66]
37. Synthesis of Some New Pyrazolo[3,4-d]pyrimidines and Pyrazolo[3,4-c]pyrazoles." V.K.Ahluwalia, Aruna Dahiya &**Madhu Bala**, *Indian J. of Chem.*, 1996, 35B, 848. [NOPR, IF-0.491]
38. A Facile One Pot Synthesis of Some New Derivatives of Pyrano[2,3-d]pyrimidines as Potential Antibacterial and Antifungal Agents". V.K.Ahluwalia &**Madhu Bala**, *Indian J. of Chem*., 1996,

35B, 742. [NOPR, IF- 0.0.491]

39. Novel Synthesis of Thieno[2,3-c]pyrazoles and Thieno[2,3-d]pyrimidines." V.K.Ahluwalia, Aruna Dahiya &**Madhu Bala**, *Indian J of Chem*., 1996, 35B, 715. [NOPR, IF:0.491]

Conference Organization/ Presentations

Organization of a Conference

1. Convener and organizing Secretary 9th**Workshop on Bioinformatics and Molecular Modeling in Drug Design,** at ACBR**,** 25-27 March, 2019
2. Convener and organizing Secretary 8th**Workshop on Bioinfromatics and Molecular Modeling in Drug Design,** at ACBR**,** 15-17 March, 2018
3. Convener and organizing Secretary 7th**Workshop on Bioinfromatics and Molecular Modeling in Drug Design,** at ACBR**,** 23-25 March, 2017
4. Registration- In- Charge, **Annual symposium on frontiers of biomedical research, ACBR,** 14-16 April 2014 and October 2015, 2016 and 2018.
5. Convener and organizing Secretary 6th**Workshop on Bioinfromatics and Molecular Modeling in Drug Design,** at ACBR**,** 21-23 January, 2016
6. Convener and organizing Secretary 5th**Workshop on Bioinfromatics and Molecular Modeling in Drug Design,** at ACBR**,** 21-23 March, 2013.
7. Convener and organizing Secretary 4th**Workshop on Bioinfromatics and Molecular Modeling in Drug Design,** at ACBR**,** 18-20 January, 2012.
8. Invited Resource Training Person at Workshop entitled, "**Bioinformatics and its applications in Drug Designing**", held at Kumaun University Nainital during 22-23 March 2011.
9. Convener and organizing Secretary **3rd Workshop on Bioinfromatics and Molecular Modeling in Drug Design,** at ACBR**,** 24-26 February 2011.
10. Drug Design and Development Using Pharmacophore Modeling and Virtual Screening at **Delhi Technological University** 23 February 2011**.**
11. Convener and organizingSecretary 2nd Workshop on Bioinfromatics and Molecular Modeling in Drug Design December, at ACBR, 22-24th 2009.

Invited Lectures= 33 since 2009

1. **'In silico drug engineering and computational drug design**', Atal Faculty Development Programme, June 28 – July 02, 2021 organised by DIPSAR, New Delhi.
2. '**Computational techniques for Mechanism based drug design and development of drugs, what next?'** at workshop on Artificial Intelligence in drug development and its implications,

02 – 04 Feb 2021, CEP, INMAS, Delhi

3. **'Computational Technologies and Drug Design Strategies',** in Summer Academic and Internship Program (SAIP)-2020, Bioescalator: Insights into Biotechnology, Plant Science and Bioinformatics, on 20th May 2020 (**Online Webinar**) organized by IILM College of Engineering and Technology, Gr. Noida.
4. 'Combination therapy of cervical cancer using lysine deacetylase (LDAC) and DNA damaging agents', in Emerging Trends in Translational Oncology on 14-15 Feb. 2020 at **AIIMS New Delhi.**
5. "Rational Drug Design and Development" in workshop on Bioinformatics and Computational Biology on June 1, 2019 at **Supercomputing Facility IIT New Delhi**
6. "Computer Aided Drug Design to reduce animal use in drug development" in National Workshop on 'Alternative methods to animal testing' on 27thto 29thMarch 2019, at **Rajguru College of Applied Sciences, New Delhi.**
7. "Mechanism Based Rational Design and Development of Drugs" in NATIONAL CONFERENCEonEmerging Trends in Computational Drug Discovery(ETCCD-2018), August 16-17, 2018, at **KIET school of Pharmacy**, Ghaziabad
8. "Computational methods for rational drug design and development" on 3rd July, 2018 at Department of Biotechnology at **IILM -CET, Greater Noida in Faculty Development Programme**, entitled *Approaches for Insilico drug designing sponsored by APJAKTU , scheduled from July 3-7, 2018.*
9. "Computer Aided Drug Design Strategies", 28th August 2017, at **Bioinformatics and Computational Biologyworkshop at IIT, New Delhi.**
10. Computer Aided Drug Design, 26th July 2017, National Faculty Development Programme **on "Recent Trends in Applied Science Teaching (FDP-RTAST)"** from 21st - 27th July, 2017 organized by Rajguru College of Applied Sciences, New Delhi
11. "Process of Drug Discovery and Development: Inventing drugs through use of Computational methods", 3rd October 2016, **Bioinformatics and Computational Biologyworkshop at IIT, New Delhi.**
12. "Synergistic effect of HDAC inhibitor (Panobinostat) and Topoisomerase inhibitors on cervical cancer at Drug **Discovery & therapy World congress,** July 22-25, 2015, **Boston, USA**
13. HDAC inhibitor and Topoisomerase inhibitors show synergistic effect on HeLa cells, **Global cancer Summit, 18-20 November, 2015**at Indian Institute of Science, JN. Tata Auditorium**, Bengaluru.**
14. "Pharmacophore based virtual screening and docking to identify novel lead compounds as potential Histone Deacetylase (HDAC) inhibitors" at Indo-Us conference on **Molecular modelling and informatics in DrugDesign 3rd-6th Nov 2014** at National Institute of Pharmaceutical Research (NIPER), Mohali Punjab.
15. "Pharmacophore-based virtual screening and docking studies to develop Histone Deacetylase (HDAC) Inhibitors" lecture in National workshop on medical bioinformatics,

December 13, 2013, MDU, Rohtak.

16. "Computer aided drug design: Strategies to discoveries", Lecture in National workshop on advances in computer aided drug design & discovery, **18-19 Oct. 2013**, Rameesh Institute Greater Noida
17. "Lead identification using pharmacophore modeling and docking as virtual screening approaches" 5th Bioinformatics Seminar cum hands-on training 2013 on Multi-Criteria Drug Design, **21-22 August 2013** , at Jamia Hamdard.
18. Lecture at Chemistry Biology Interface, **May 2013**, held at Dyal Singh College, Delhi University.
19. Basics of Bioinformatics and structure based drug design in National Seminar cum workshop on applications of Bioinformatics in Life Sciences at Jiwaji University on **08-09th March 2013**
20. Lead Identification Using Pharmacophore Modeling & Virtual Screening inSymposium on Bioinformatics at DRDE Gwalior, during **22-24, August 2012**
21. "Protein Homology modeling and structure based drug Design", at Computational biology workshop at **Miranda House**, **January 2012**.
22. *"Computational Drug Design and Development" at workshop entitled Computational*. Chemistry for Chemistry Educators at **Miranda House***,* 23-24, Nov, *2011*
23. Mechanism Based Drug Design and Development Using Computational Methods, Workshopat **Acharya Narendra Dev College**, 4 March 2011.
24. Mechanism Based Drug Development: Using Computational Methods for Developing Target Based Therapeutics at National Conference on Recent **Advances in Pure and Applied Chemistry**, ACBR, Delhi, 28-29 December 2010
25. Drug Design and Development Using Pharmacophore Modeling and Virtual Screening at **Delhi Technological University,** 23 February 2011**.**
26. Drug Design And Development Using Pharmacophore Modeling And Virtual Screeningat **International Conference & Exhibition on Analytical & Bioanalytical Techniques 2010: Pharmaceutical R & D Summit,** Hyderabad, November 1-3 2010.
27. Drug Design and Development Using Computational Methods, Workshop on **Bioinformatics** at Maharishi Dayanand University Rohtak, 15th September 2010
28. Drug Design and Development Using Computational Methods, **Training Programme in Bioinformatics and Drug Design,** at IIT Delhi 30th August 2010.
29. Mechanism Based Drug Development: Using Computational Methods for Developing Target Based Therapeutics, **Workshop on INMAS-DU Collaboration**, 20th August 2010, at INMAS, Delhi.
30. Drug Design & Development - Modeling at **National Workshop on Computational Science**, held at the Department of Physics& Astrophysics & DUCCC, University of Delhi. 1-7, July 2010

31. Drug Design And Development Using Pharmacophore Modeling And Virtual Screening at **National Conference on Medical Biotechnology vision -2020**, April 16-18, 2010
32. Design And Development Of Cyclooxygenase-2 Inhibitors Using Pharmacophore Modeling And Virtual Screening at International Conference **on Trends in Drug Discovery and Development (T3D-2010)**, 5-8 January 2010, Department of Chemistry, University of Delhi.
33. Mechanistic study of Inhibition of human cervical tumour cell growth by Etoricoxib, a highly selective COX-2 inhibitor at **World Cancer Congress (WCC-2009)**, 12-14 January 2009, Kottayam Kerala.

Poster Presentation by Students26

Research Projects (Major Grants/Research Collaboration)

Award: Drug Discovery Hackathon Phase I- Award (DDH-2020), open source drug discovery Hackathon against Covid-19, Organised by Innovation Cell, Ministry of Education also selected for Phase II project.

Ongoing Project

1. BIC project, entitled "Drug Development: From Target Identification, Validation to Drug discovery- BIC of Dr. B. R. Ambedkar Center for Biomedical Research, University of Delhi, Delhi". **Rs. 189.36 Lakhs**. Sanctioned in 2020-21., DBT, duration 5 years
2. "Screening of novel molecules for drug re-purposing for development of antiviral therapeutics against COVID19", FRP, University of Delhi, Rs. 3 Lakhs, 2021-22
3. Drug repurposing using computer aided design for development of antiviral compounds against COVID19: *in silico* and *in vitro* Screening against selected antiviral targets, Institute of Excellence, FRP, University of Delhi, **Rs. 5 lakhs**, 2020-21
4. Targeted screening of hit molecules and modulation of lead compounds for clinical management of covid 19: in vitro and antiviral evaluation, Drug Discovery Hackathon Phase II, MHRD INNOVATION CELL, **Rs. 23 lakhs**, 2021-22
5. Screening of novel molecules for drug re-purposing for development of antiviral therapeutics against COVID19, Institute of Excellence, FRP, University of Delhi, Rs. 3 lakhs, 2020-21

Project Submitted to DBT and passed through Technical Committee (under consideration)

6. National Network Project of Dr. B. R. Ambedkar Center for Biomedical Research, University of Delhi, Delhi. Rs. 200 Lakhs (**FILE NUMBER – 40195)**

Completed Projects:

Total Research Grants obtained = Rs. **2.03crores** (7 major projects as PI)

DU-R & D projects = Rs. **20 lakhs** (2008-2016; as PI)

Departmental projects (Co-PI) = Rs. **1.5 Crores** (DU-DST PURSE)

Rs. **35 lakhs** (UGC-SAP I)

Rs. **1.5 crores** (UGC-SAP II)

- **Completed (Major Projects) =** 09 **(More than 4 lakhs)**
- **Completed (Minor Projects) =** 08 **(less than 4 lakhs)**

Details

- **Creation of Bioinformatics Infrastructure Facility (BIF) at ACBR,** Institutional **Project Coordinator& PI**: Madhu Chopra. Since 2006- 2019(Total sanctioned till 2019 = **Rs. 1.04 Crores**)
- DU-DST Purse grant phase II, sanctioned **Rs. 1.5 crore** to ACBR, ***co-investigator*** with other faculty members.
- UGC-SAP project, Sanctioned **Rs. 1.5 Crore** to ACBR, ***Co-investigator*** with other faculty members.
- "Development of Anticancer Therapeutics: Targeting drug loaded nanocarriers to CD44, A Hyaluroan Receptor" Sanctioned by University of Delhi under DST-PURSE scheme, **Rs. 12.89 Lakhs**, 2009-september 2013, Madhu Chopra (**PI)**
- Structure Based Design, Synthesis and Evaluation of Histone Deacetylase Inhibitors as Potent Antitumour Agents, Sanctioned by DBT, **Rs. 11.68 Lakhs**, June **2009-2011,** Madhu Chopra (**PI**), Anil Mishra & Aruna Chhikara (Co-PI)
- Delhi University Special Grant for Research Work**, Rs. 20 Lakhs Approx**, **2008, 2009, 2010, 2011, 2012, 2013, 2014, 2015.**
- Isolation, Chemical Characterization and Biological evauation of Potential Anticancer Agents From *Boerhavia diffusa* Project Proposal sanctioned by **ICMR (Rs. 11 Lakhs),** October 2006. Dr. Madhu Chopra (**PI**), Dr. Daman Saluja (CO-PI)
- Computer-Aided Design of Novel NSAIDs as Selective Cyclooxygenase-2 (COX-2) inhibitors to target tumors: Pilot Study for Synthesis and Preliminary Activity for its Anti-tumor Potential Investigators: Dr Madhu Chopra (**PI**) & Dr. Daman Saluja (CO-PI)Sanctioned by *DBT*, 2005-2009

(**Rs. 30 + 7 Lakhs** (Extension for one year)

- Synthesis and Evaluation of ^{99m}Tc-Ciprofloxacin Analogues for Infection Imaging. Project Proposal sanctioned by**INMAS, DRDO(Rs. 8 Lakhs)**Dr. Madhu Chopra (**PI)** , Dr. Daman Saluja (CO-PI) & Dr. A. K. Mishra , INMAS (CO-PI)
- Design, Synthesis and Evaluation of non Peptidic CCK-B receptor Specific Antagonists for targeting CCK-B receptor expressing Tumours. Dr. Madhu Chopra (**Principal Investigator**), Prof. Vani Brahmachari & Dr. Anil Mishra. Sanctioned **by DST (Rs. 18 Lakhs**)

Mentoring following projects:

- Combination therapy of gastric cancer- combining HGF with HDAC- PI-Dr. Rakhi Srivastava. Sanctioned by MOHFW **2018-20**, Rs. 30 Lakhs
- Design and development of novel inhibitors of AKR1C1 as potential late candidates in treatment of breast, cervical and endometrial cancers; PI Dr. Priyanka Verma. Sanctioned by MOHFW **2016-19**, Rs. 30 Lakhs

COLLABORATIVE PROJECTS

- **Biodegradable** nanoparticle based drug delivery Systems, Sanctioned by UGC, PI- Aruna Chhikara, Co-PI – Madhu Chopra, Rs. **7 lakhs**Development of Radiopharmaceutical for targeted drug Delivery with **Dr. Anil K. Mishra**, INMAS.
- Biodegradable Nanogels as Potential Drug Delivery Carriers for Development of Target Specific Chemotherapeutic Agents Dr. Aruna Chhikara (PI), Madhu Chopra (CO-PI), Sanctioned **from UGC , 2008 (Rs. 6 lakhs)**
- Collaboration with **Dr. Krishana Dalal, AIIMS** " Estimation of the level of Cartilage Oligomeric Matrix protein (COMP) in Osteoarthritis and Designing of an Inhibitor to control the progression of Osteoarthritis"
- Collaboration with prof. Veena Agarwal, Department of Botany, University of Delhi
- Ms. Ruby Gupta, visited to **Prof. J. R. Dimmock** Laboratory as GSEP Scholar At Drug Design and Discovery Group, University of Saskatchewan, Saskatoon, Canada (December 2009-August 2010)
- Computational design and prediction of activity of novel opioid receptor antagonists and antitensin converting enzyme inhibitors with **Dr. Santosh Pasha, IGI**B (2008-2013).

Awards and Distinctions

- Drug Discovery Hackathon Phase I- Award (DDH-2020), open -source drug discovery Hackathon against Covid-19, Organised by Innovation Cell, Ministry of Education.
- Research Associateship, C.S.I.R., New Delhi (April 1996- Oct. 1997)
- Senior Research Fellowship, U.G.C., New Delhi (Jan. 1995- Dec. 1995)
- Junior Research Fellowship, U.G.C., New Delhi (Jan. 1993- Dec. 1994)

Association with Professional Bodies

Reviewing

1. Journal of Experimental & Clinical Cancer Research (BMC-Springer Nature)
2. Molecular and Cellular Biochemistry (Springer)
3. Journal of Chemical Information and Modeling (American Chemical Society)
4. Biotechnology Progress, American Institute of Chemical Engineers (AIChE)
5. Antiviral research (Elsevier)
6. European Journal of Medicinal Chemistry (Elsevier)
7. AAPS PharmSciTech (American Chemical Society)
8. Molecular Medicine (BMC-Springer Nature)
9. Indian Journal of Biophysics and Biochemistry
10. Project Reviewing for DBT, DRDO and ICMR.

Memberships

- American Chemical Society Membership
- LIFE MEMBER Indian Science Congress Association
- LIFE MEMDER Indian Association for Cancer Research

Other Activities

Signature of Faculty Member
Date: 23/03/2022