Curriculum Vitae

Dr. Durgesh Kumar
DOB: 15 January, 1989
Ph.D., Department of Chemistry,
University of Delhi, New Delhi-110007, India
Phone: +91-9599533822, 9818742116.
Email: durgeshrawat1989@gmail.com, dkumar1@maitreyi.du.ac.in

Educational Qualification:-

- I have done Ph.D. entitled "**Oxazolidine based nsP3 Protease of CHIKV Inhibitor: Designing, Virtual Screening, Docking and Molecular Dynamics Simulations**" on February 2021, at Department of Chemistry, University of Delhi, New Delhi India 110007 under the supervision of **Prof. Prashant Singh**.
- I have published more than 28 research articles in reputed journals with more than 90 impact factor and 430 citations.
- MD simulations was done at SCFBio, IIT Delhi in the research group of **Prof. B. Jayaram.**
- M. Sc. in **Applied Chemistry** from Babasaheb Bhimrao Ambedker University, (A Central University) Lucknow, U.P. India in 2013.
- B. Sc. in **Chemistry & Botany** from University of Lucknow, U.P. India in 2011.

Achievements:-

- **First position** in oral presentation in the International conference *"Recent trends in drug discovery and development"* department of Chemistry (Under the aegis of IQAC) Maitreyi College, University of Delhi, Chanakyapuri, New Delhi on October 8-9, 2021
- **Junior Research Fellow (January, 2016 – December, 2017):** Council of Scientific & Industrial Research (CSIR), New Delhi, India.
- **Senior Research Fellow (January 01, 2018 – August 09, 2020):** Council of Scientific & Industrial Research (CSIR), New Delhi, India.
- **Qualified** Graduate Aptitude Test in Engineering (GATE) February 2016.
- **Qualified** Council of Scientific & Industrial Research – Junior Research Fellow (CSIR-JRF) in June 2016 conduct by CSIR, New Delhi, India.

- **Qualified** Council of Scientific & Industrial Research – Junior Research Fellow (CSIR-JRF) June 2015 conduct by CSIR, New Delhi, India.
- **Qualified** Council of Scientific & Industrial Research – National Eligibility Test (CSIR-NET Lectureship) December 2013 conduct by CSIR, New Delhi, India.

Research and Professional Experience:-

- Working as Assistant Professor in Maitreyi College, University of Delhi at undergraduate level from 24 November, 2020 to till now.
- Worked as Assistant Professor in Lady Irwin College, University of Delhi at undergraduate level from 10 August, 2020 to 23 November, 2020.
- Worked as Assistant Professor in Lady Irwin College, University of Delhi at undergraduate level from 20 August, 2019 to 19 November, 2019.

I have also worked on the inhibition of nsP3 and nsP2 of CHIKV along with COVID-19.

International Publications:-

1. Aslam, M.; Singh, M. B.; Singh, P.; Pandey, G.; Kumar, A.; Singh, S.; Tumba, K.; Chopra, H.; **Kumar, D.;** Kumari, K. Impact of functional group positioning in the anion of ionic liquids on aqueous solubility: a study through DFT calculations in *Ionics (Springer Berlin Heidelberg)*, November 28, **2023**, 1-13. (**Impact Factor**: 2.961).
2. Raman, A. P. S.; Pongpaiboon, S.; Bhatia, R.; Dabodhia, K. L.; Kumar, A.; **Kumar, D.;** Jain, P.; Sagar, M.; Singh, P.; Kumari, K. *In silico* study on antidiabetic and antioxidant activity of bioactive compounds in Ficus carica L *in Journal of Biomolecular Structure and Dynamics*, August 6, **2023**, 41 1-17. (**Impact Factor**: 5.235).
3. **Kumar, D.;** Kumari, K.; Chandra, R.; Jain, P.; Vodwal, L.; Gambhir, G.; Singh, P. A review targeting the infection by CHIKV using computational and experimental approaches in *Journal of Biomolecular Structure and Dynamics*. **2022**, 1-15. (**Impact Factor**: 5.235)
4. Singh, M. B.; Sharma, R.; **Kumar, D.;** Khanna, P.; Mansi., Khanna, L.; Kumar, V.; Kumari, K.; Gupta, A.; Chaudhary, P.; Kaushik, N.; Choi, E. W.; Kaushik, N. K.; Singh, P. An understanding of coronavirus and exploring the molecular dynamics

simulations to find promising candidates against the Mpro of nCoV to combat the COVID-19: A systematic review in *Journal of Infection and Public Health,* **2022**, 15, 1326-1349. (**Impact Factor**: 7.7)

5. Meena, M. K.; **Kumar, D.;** Kumari, K.; Kaushik, N. K.; Kumar, R. V.; Bahadur, I.; Vodwal, L.; Singh, P. Promising inhibitors of nsp2 of CHIKV using molecular docking and temperature-dependent molecular dynamics simulations in *Journal of Biomolecular Structure and Dynamics*. **2022**, 40 (13), 5827-5835. (**Impact Factor**: 5.235)
6. Kumar, A.; **Kumar, D.;** Kumar, R.; Singh, P.; Chandra, R.; Kumari, K. DFT and docking studies of designed conjugates of noscapines & repurposing drugs: promising inhibitors of main protease of SARS-CoV-2 and falcipan-2 in *Journal of Biomolecular Structure and Dynamics*. **2022**, 40 (6), 2600-2620. (**Impact Factor**: 5.235)
7. Meena, M. K.; **Kumar, D.;** Jayaraj, A.; Kumar, A.; Kumari, K.; Katata-Seru, L.; Bahadur, I.; Kumar, V.; Sherawat, A.; Singh, P. Designed thiazolidines: An arsenal for the inhibition of nsP3 of CHIKV using molecular docking and MD simulations in *Journal of Biomolecular Structure and Dynamics*. **2022**, 40 (4), 1607-1616. (**Impact Factor**: 5.235)
8. Singh, P.; **Kumar, D.;** Pal, S.; Kumari, K.; Bahadur, I. L-amino-acids as immunity booster against COVID-19: DFT, molecular docking and MD Simulations in *Journal of molecular structure*. **2022**, 1250, 131924. (**Impact Factor**: 3.841)
9. **Kumar, D.;** Meena, M. K.; Kumar, V.; Singh, P.; Bahadur, I., Impact of Temperature on Structural Changes in nsp2 and nsp3 of CHIKV: Molecular Dynamics Simulations in *Research Square.* **2022,** 1-9.
10. Kumar, A.; Kumari, K.; Raman, A. P. S.; Jain, P.; **Kumar, D.;** Singh, P. An insight for the interaction of drugs (acyclovir/ganciclovir) with various ionic liquids: DFT calculations and molecular docking in *Journal of Physical Organic Chemistry*. **2022**, 35 (1), e4287. (**Impact Factor**: 2.155)
11. **Kumar, D.;** Kumari, K.; Vishvakarma, V. K.; Jayaraj, A.; Kumar, D.; Ramappa, V. K.; Patel, R.; Kumar, V.; Dass, S. K.; Chandra, R. Promising inhibitors of main protease of novel corona virus to prevent the spread of COVID-19 using docking and molecular dynamics simulation in *Journal of Biomolecular Structure and Dynamics*. **2021,** *39* (13), 4671-4685. (**Impact Factor**: 5.235)

12. **Kumar, D.;** Meena, M.; Kumari, K.; Kumar, R.; Bahadur, I.; Jain, P.; Singh, P. Exploring the effect of temperature on inhibition of non-structural protease 3 of Chikungunya virus using molecular dynamics simulations and thermodynamics parameters in *Journal of Molecular Liquids.* **2021,** *335*, 116164. (**Impact Factor**: 6.633)
13. **Kumar, D.;** Kumari, K.; Jayaraj, A.; Kumar, V.; Kumar, R. V.; Dass, S. K.; Chandra, R.; Singh, P. Understanding the binding affinity of noscapines with protease of SARS-CoV-2 for COVID-19 using MD simulations at different temperatures in *Journal of Biomolecular Structure and Dynamics*. **2021,** *39* (7), 2659-2672. (**Impact Factor**: 5.235)
14. Kumar, A.; **Kumar, D.;** Kumari, K.; Mkhize, Z.; Katata Seru, L. M.; Bahadur, I.; Singh, P. Metal-ligand complex formation between ferrous or ferric ion with syringic acid and their anti-oxidant and anti-microbial activities: DFT and molecular docking approach in *Journal of Molecular Liquids*. **2021**, 322, 114872. (**Impact Factor**: 6.633).
15. Kumari, K.; **Kumar, D.;** Kumar, R. V.; Singh, P. Kuwanons, promising inhibitors against the ACE-2, main protease of SARS-CoV-2 and falcipan-2 using molecular docking in *Research Square*. **2020**, 1-15
16. **Kumar, D.;** Kumari, K.; Bahadur, I.; Singh, P., Promising Acyclovir and its derivatives to inhibit the protease of SARS-CoV-2: Molecular Docking and Molecular Dynamics simulations in *Research Square***. 2020,** 1-17.
17. **Kumar, D.;** Kumari, K.; Singh, P., A Theoretical Model to Study the Interaction Between Boronic Acids and Insulin in *ChemRxiv*. **2020,** 1-14.
18. **Kumar, D.;** Meena, M. K.; Kumari, K.; Patel, R.; Jayaraj, A.; Singh, P. In-silico prediction of novel drug-target complex of nsp3 of CHIKV through molecular dynamic simulation in *Heliyon*. **2020,** *6* (8), e04720. (**Impact Factor**: 3.776)
19. **Kumar, D.;** Kumari, K.; Jayaraj, A.; Singh, P. Development of a theoretical model for the inhibition of nsP3 protease of Chikungunya virus using pyranooxazoles in *Journal of Biomolecular Structure and Dynamics*. **2020,** *38* (10), 3018-3034. (**Impact Factor**: 5.235)
20. **Kumar, D.;** Singh, P.; Jayaraj, A.; Kumar, V.; Kumari, K.; Chandra, R.; Ramappa, V. K. Selective Docking of Pyranooxazoles Against nsP2 of CHIKV Eluted Through Isothermally and Non-Isothermally MD simulations in *ChemistrySelect*. **2020,** *5* (14), 4210-4220. (**Impact Factor**: 2.307)

21. Azad, I.; Akhter, Y.; Khan, T.; Azad, M. I.; Chandra, S.; Singh, P.; **Kumar, D.;** Nasibullah, M. Synthesis, quantum chemical study, AIM simulation, in silico ADMET profile analysis, molecular docking and antioxidant activity assessment of aminofuran derivatives in *Journal of Molecular Structure*. **2020,** *1203*, 127285. (**Impact Factor**: 3.841)
22. Singh, P.; **Kumar, D.;** Vishvakarma, V. K.; Yadav, P.; Jayaraj, A.; Kumari, K. Computational approach to study the synthesis of noscapine and potential of stereoisomers against nsP3 protease of CHIKV in *Heliyon*. **2019,** *5* (12). (**Impact Factor**: 3.776).
23. **Kumar, D.;** Singh, P.; Jayaraj, A.; Kumar, V.; Kumari, K.; Patel, R. A theoretical model to study the interaction of erythro-noscapines with nsP3 protease of Chikungunya virus in *ChemistrySelect*. **2019,** *4* (17), 4892-4900. (**Impact Factor**: 2.307).
24. Singh, P.; Kumari. K.; Vishvakarma, V. K.; Mehrotra, G. K.; Chandra, R.; **Kumar, D.;** Patel, R.; Shahare, V. V. Metal NPs (Au, Ag and Cu): Synthesis, Stabilization and their Role in green chemistry and drug Delivery in *Springer International Publishing AG*. **2017,** *1*, 309-337. (**Impact Factor**: 3.182).
25. **Kumar, D.;** Kumari, K.; Vishvakarma, V. K.; Singh, P.; Chandra, R.; Athar, M. Sulphonylurea, Metformin, TZDs: Potential drugs to cure Diabetes in *International J. Advanced Biomed.* 2017, 1, 11-18. (**Impact Factor**: 0.034).
26. **Kumar, D.;** Singh, P.; Chandra, R.; Kumari, K.; Kumar, M. Impact of Gemini Surfactants on the stability of Insulin using computational tools in *J Nanomed Biother*. **2017,** *7*, 1-5. (**Impact Factor**: 3.687)
27. **Kumar, D.;** Athar, M.; Kumar, G. Methods And Techniques Employed For Sugar Decolorization in *LAP LAMBERT Academic Publishing.* **2014,** *1*, 1-72.

Posters presented in national/ international conference:-

1. Poster presentation in ‘‘National Seminar on Biophysika” at centre for interdisciplinary research in basic science **Jamia Millia Islamia**, New Delhi 110025 on 20 November **2018.**
2. Poster presentation in “Recent Frontiers in Chemistry” in Department of Chemistry, **HNB Garhwal University,** Srinagar Garhwal – 246174 Uttarakand from 27th-28th April,**2018**.

3. Poster presentation in "National Science Day 2018" jointly organized by Indian Academy of Science, Bangalore and Indian National Science Academy, Delhi on 28 February **2018** at **INSA** Delhi, India.
4. Poster presentation in *"*Recent Advance in Chemical Sciences towards Green & Sustainable Environment: Swachh Bharat Abhiyan Perspective" at **Aditi Mahavidyalaya** (University of Delhi) New Delhi on 10-11 Oct. **2017.**
5. Poster presentation in *"*National Seminar on Biophysics" at centre for interdisciplinary research in basic science **Jamia Millia Islamia**, New Delhi 110025 on**2017.**
6. Presented poster in **"**Trendsin Research and Innovations in Life Sciences" at Undergraduate level" in **DDU College University of Delhi** on 30 March **2016**.

Conference/ workshop attended:-

1. Oral presentation in "sustainable Future for Humanity: The new learning curve" at Maitreyi College, University of Delhi, New Delhi, India on 24 February, 2021.
2. Participated in one week national online FDP jointly organized by Guru Angad Dev Teaching Learning Centre, SGTB Khalsa College, University of Delhi, New Delhi, India from 15 December, 2021 to 21 December, 2021.
3. Participated in "Bioinformatics Workshop on Genomics, Proteomics, Drug Design and High Performance Computing" at the Supercomputing Facility for Bioinformatics and Computing Biology, **Indian Institute of Technology Delhi** from 8^{th}-14^{th} December **2018**.
4. Participated in "One day workshop on Molecular Modelling" at **Atma Ram Sanatan Dharma College**, University of Delhi, New Delhi on 3^{rd} January **2018**.
5. Participated in "One day workshop on Archival Sciences" at **Atma Ram Sanatan Dharma College**, University of Delhi, New Delhi on 20 February **2018**.
6. Participated in "One day Faculty Development Programme" at **Atma Ram Sanatan Dharma College**, University of Delhi, New Delhi on 10^{th} November **2017**.

Research Summary

Aim of my Ph.D. work was based on *in silico* drug design to find potential drug molecules against nsP3 protease of CHIKV. From the literature survey, it is found that derivatives of Oxazolidine are a class of synthetic antibacterial agents that act as a protein synthesis inhibitor on the ribosomal 50S subunit of the bacteria.

Oxazolidine-2, 4-dione is a compound that forms the core structure of a variety anticonvulsant drugs including Dimethadione, Ethadione, Paramethadione and Trimethadione. Oxazolidines were used for the treatment and prevention of metabolic bone disorders, anticancer agent against A549 (lung) and DU145 (prostate) cancer cells, muscle relaxants, good activity against bacterial as well viral infections. For this study, I have designed five chemical reactions using oxazolidine-2, 4-dione (OZD) to get potential molecules based on literature knowledge. In general, these chemical reactions are based on one-pot multicomponent reactions (MCRs) that rearrangement of atoms of the reactants to create a novel molecules i.e., product molecules.

Designing: Drug libraries are collections of molecules which are designed to interact with target proteins, frequently a family of nsP3 protease of CHIKV. The designing process starts with the selection of a suitable scaffold, to which recognition of substituents or side chains. It was designed 200 molecules of each scheme by changing the alkyl groups (R_1, R_2, R_3, R_4 & R_5) in benzaldehyde moiety to get 1000 drug molecules that are derivatives of product molecules through ChemDraw and Marvin Sketch.

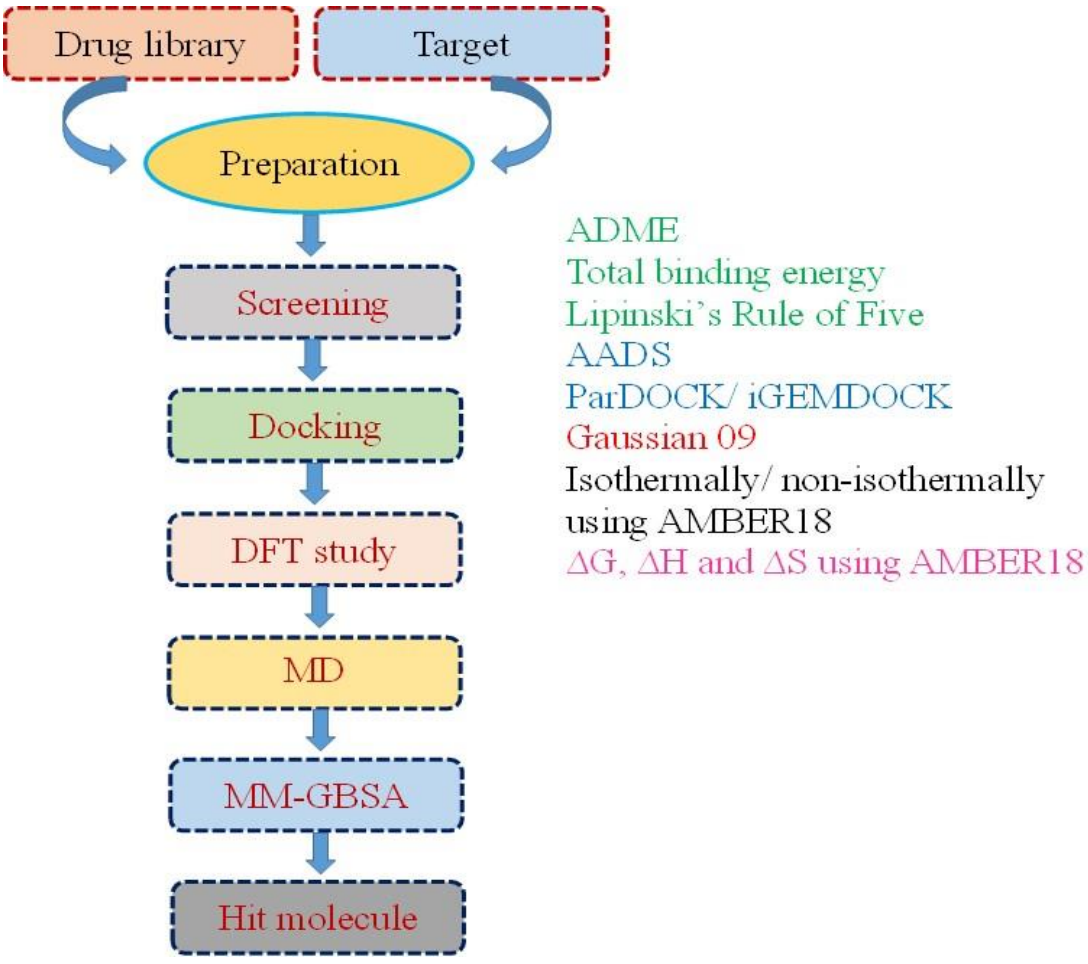
Screening: Virtual screening protocol were used to screen drug libraries from designed databases. It depends on the aim and on the knowledge availability for nsP3 protease of CHIKV target protein. Further, the activity of top hit drug molecules were studied through ADME properties.

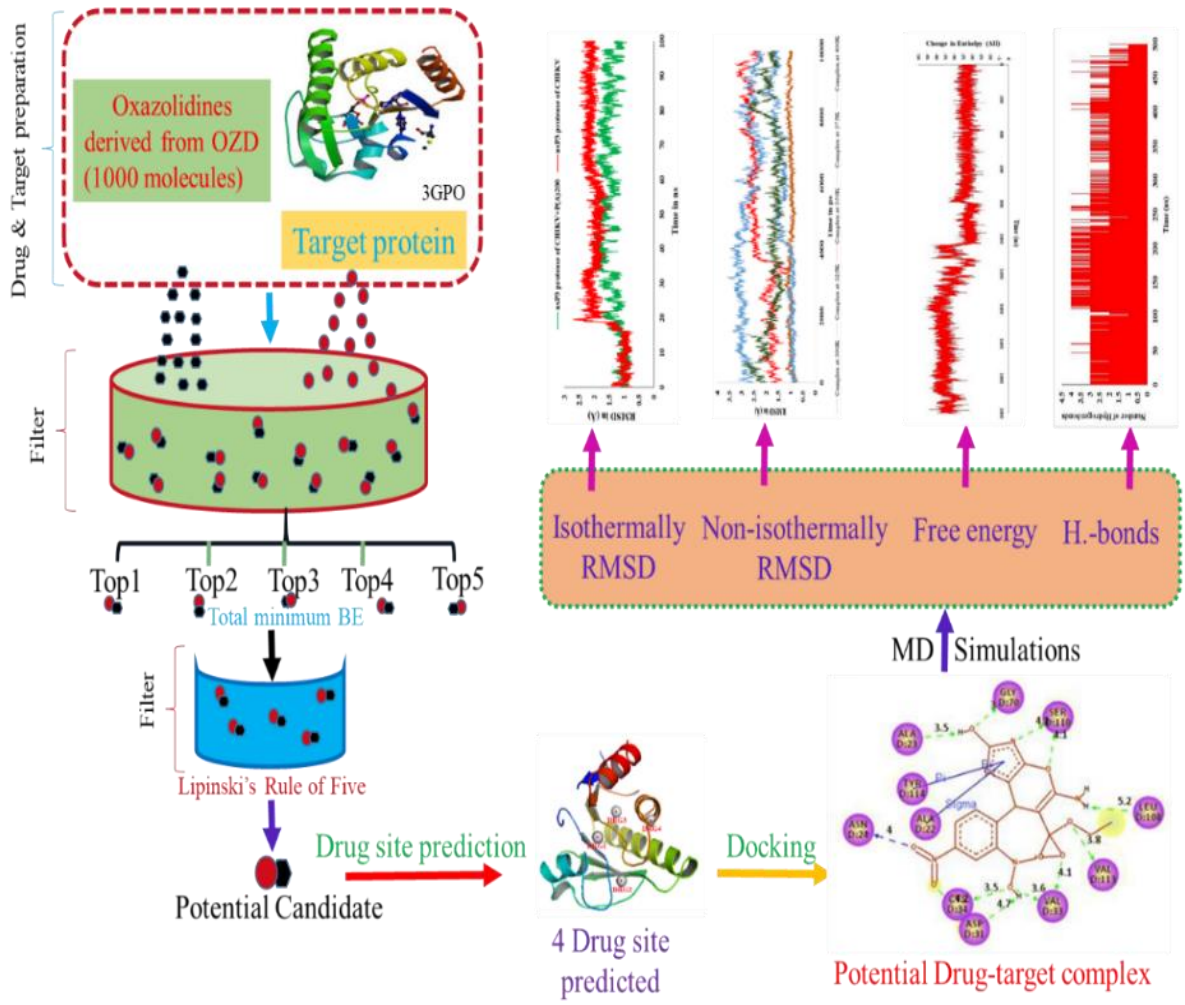
Docking: It is used to predict the binding strength of protein-ligand complex between two molecules using ParDOCK. This studies were performed using ParDOCK web server which is available on SCFBio-iitd.res.in from IIT Delhi India.

Molecular Dynamics Simulations: The Molecular Dynamics simulations of nsP3 protease of CHIKV with and without drug molecules were performed with pmemd modules of AMBER18 suite, utilizing the ff14SB force field at isothermally and non-isothermally.

MM-GBSA Method: Using MM-GBSA method to calculate relative change in binding free energy of complex system with and without drug molecules. From trajectories of MD simulation, the relative binding energy terms of complex, target, drug and difference in drug-target-complex at 100 ns, 500 ns and 2000 ns are calculated by the given equations.

DFT Study: Through density function theory (DFT), it was used to calculate the LUMO - HOMO energy gap (ΔE) or E_{Gap} from B3LYP method with the basis set 6-311G* using Gaussian. By using E_{HOMO} and E_{LUMO} energy values for top five hit drug molecules to calculate electronic terms such as chemical potential (μ), global electronegativity (χ) and chemical hardness (η) global electrophilicity (ω) respectively were estimated based on **Equation** as given below.





Hands on Computational tools to develop biologically potential candidates:-

Computational tools	Applications
ChemDraw and Marvin Sketch	It is the drawing tool of choice for chemists to create or design compound library.
iGEMDOCK	It is an integrated and easy to use environment which is especially useful for post-screening analysis and inferring pharmacological interactions from screening compounds.
RASPD	A web server for preliminary screening of drug molecules from ZINC database and screening from designed compound libraries on the basis of binding affinity (ΔG).
Gaussian 09	It is used for geometry optimization, transition state, intermediate, HOMO-LUMO gap and reaction mechanism study through DFT theory.
Notepade++;	It was used for the preparation of target protein and adding of some missing atoms/ions and removal of some extra atoms/ions.

AADS	Active site or drug site on target protein was predicated by AADS web server.
ParDOCK	It is used for selective or rigid docking of drug molecules into the cavity of target protein.
Pymol; MMV; Chemira; LigPlus; Discovery Studio.	These are computer based software, a molecular visualization system and it can produce high-quality 3D images of small molecules, biological macromolecules, such as proteins and drug-target complex systems.
Gusar; Swiss ADME; Molinspiration	A web server for prediction of Acute toxicity and biological activity score of top screened molecules.
AMBER18	Amber is a suite of bio-molecular simulation programs and it was used to simulate drug-target complex and also predicted binding affinity of drug-target complex through MM-GBSA method.

References

Prof. Prashant Singh (Supervisor)
Department of Chemistry, University of Delhi
Atma Ram Sanatan Dharma College,
Dhaula Kuan, New Delhi-110021, India
Contact No.: +91-9953622478
Email- arsdchemistry@gmail.com

Prof. Gajanan Pandey
Head, Department of Chemistry
Department of Chemistry, School of Physical & Decision Sciences Babasaheb Bhimrao Ambedkar University (a central University) (BBAU)
Lucknow-226025 (U.P.) India
Email: pandeygajanan@rediffmail.com, pandeygajanan@bbau.ac.in
Mobile: +918765583117

Prof. B. Jayaram
Professor, Department of Chemistry & Professor, Kusuma School of Biological Science, IIT Delhi-110016, India.
Coordinator, Supercomputing Facility for Bioinformatics & Computational Biology, IIT Delhi-110016, India.
Contact No.: +91-11-26591505; 26596786
Email: bjayaram@chemistry.iitd.ac.in

Prof. Indra Bahadur
Department of Chemistry, Faculty of Natural and Agricultural Sciences, North-West University, South Africa
bahadur.indra@nwu.ac.za

Declaration:

I hereby declare that the particulars furnished herein by me are true to the best of my knowledge and belief**.**

Place: New Delhi
(Dr. Durgesh Kumar)