

## Mr. IQRAR AHMAD

### Academic Qualifications

Degree	Year	University/Board	Percentage	Class
<b>B. Pharm</b>	2016	NMU, Jalgaon	70.70	Distinction
<b>M. Pharm</b>	2018	NMU, Jalgaon	76.61	Distinction
<b>PhD.</b>	2021	NMU, Jalgaon	Pursuing	-

### Research Area

EGFR tyrosine kinase inhibitors to overcome the problem of mutation and resistance in non-small cell lung cancer (NSCLC)

### Publication

**National: 00**

**International: 98**

1. Patel, H., Ansari, A., Pawara, R., Ansari, I., Jadhav, H., & Surana, S. (2018). Design and synthesis of novel 2,4-disubstituted aminopyrimidines: reversible non-covalent T790M EGFR inhibitors. *Journal of receptor and signal transduction research*, 38(5-6), 393–412. <https://doi.org/10.1080/10799893.2018.1557207>
2. Patel, H., Jadhav, H., Ansari, I., Pawara, R., & Surana, S. (2019). Pyridine and nitro-phenyl linked 1,3,4-thiadiazoles as MDR-TB inhibitors. *European journal of medicinal chemistry*, 167, 1–9. <https://doi.org/10.1016/j.ejmech.2019.01.073>
3. Patel, H., **Ahmad, I.**, Jadhav, H., Pawara, R., Lokwani, D., & Surana, S. (2020). Investigating the Impact of Different Acrylamide (Electrophilic Warhead) on Osimertinib's Pharmacological Spectrum by Molecular Mechanic and Quantum Mechanic Approach. *Combinatorial chemistry & high throughput screening*, 10.2174/1386207323666201204125524. Advance online publication. <https://doi.org/10.2174/1386207323666201204125524>
4. Patel, H. M., **Ahmad, I.**, Pawara, R., Shaikh, M., & Surana, S. (2021). In silico search of triple mutant T790M/C797S allosteric inhibitors to conquer acquired resistance problem in non-small cell lung cancer (NSCLC): a combined approach of structure-based virtual screening and molecular dynamics simulation. *Journal of biomolecular structure & dynamics*, 39(4), 1491–1505. <https://doi.org/10.1080/07391102.2020.1734092>
5. Patel, H. M., Shaikh, M., **Ahmad, I.**, Lokwani, D., & Surana, S. J. (2021). BREED based

- de novo hybridization approach: generating novel T790M/C797S-EGFR tyrosine kinase inhibitors to overcome the problem of mutation and resistance in non small cell lung cancer (NSCLC). *Journal of biomolecular structure & dynamics*, 39(8), 2838–2856. <https://doi.org/10.1080/07391102.2020.1754918>
6. **Ahmad, I.**, Shaikh, M., Surana, S., Ghosh, A., & Patel, H. (2020). p38 $\alpha$  MAP kinase inhibitors to overcome EGFR tertiary C797S point mutation associated with osimertinib in non-small cell lung cancer (NSCLC): emergence of fourth-generation EGFR inhibitor. *Journal of biomolecular structure & dynamics*, 1–14. Advance online publication. <https://doi.org/10.1080/07391102.2020.1844801>
7. **Ahmad, I.**, Jadhav, H., Shinde, Y., Jagtap, V., Girase, R., & Patel, H. (2021). Optimizing Bedaquiline for cardiotoxicity by structure based virtual screening, DFT analysis and molecular dynamic simulation studies to identify selective MDR-TB inhibitors. *In silico pharmacology*, 9(1), 23. <https://doi.org/10.1007/s40203-021-00086-x>
8. **Ahmad, I.**, Kumar, D., & Patel, H. (2021). Computational investigation of phytochemicals from *Withania somnifera* (Indian ginseng/ashwagandha) as plausible inhibitors of GluN2B-containing NMDA receptors. *Journal of biomolecular structure & dynamics*, 1–13. Advance online publication. <https://doi.org/10.1080/07391102.2021.1905553>
9. Extensively Drug-resistant Tuberculosis (XDR-TB)-inhibitors to Overcome the Scourge of Drug-resistant Tuberculosis: a Perspective Review *Journal of Chemistry, 2020, Vol. 10, No. 3–4, pp. 112–139.* <https://doi.org/10.1134/S2079978020030048>
10. Jagatap, V. R., **Ahmad, I.**, & Patel, H. M. (2022). Recent updates in natural terpenoids as potential anti-mycobacterial agents. *The Indian journal of tuberculosis*, 69(3), 282–304. <https://doi.org/10.1016/j.ijtb.2021.07.006>
11. Shinde, Y., **Ahmad, I.**, Surana, S., & Patel, H. (2021). The Mur Enzymes Chink in the Armour of Mycobacterium tuberculosis cell wall. *European journal of medicinal chemistry*, 222, 113568. <https://doi.org/10.1016/j.ejmech.2021.113568>
12. Shaikh, M., Shinde, Y., Pawara, R., Noolvi, M., Surana, S., **Ahmad, I.**, & Patel, H. (2021). Emerging Approaches to Overcome Acquired Drug Resistance Obstacles to Osimertinib in Non-Small-Cell Lung Cancer. *Journal of medicinal chemistry*, 10.1021/acs.jmedchem.1c00876. <https://doi.org/10.1021/acs.jmedchem.1c00876>
13. Pawara, R., **Ahmad, I.**, Nayak, D., Wagh, S., Wadkar, A., Ansari, A., Belamkar, S., Surana, S., Nath Kundu, C., Patil, C., & Patel, H. (2021). Novel, selective acrylamide linked quinazolines for the treatment of double mutant EGFR-L858R/T790M Non-Small-Cell lung cancer (NSCLC). *Bioorganic chemistry*, 115, 105234. <https://doi.org/10.1016/j.bioorg.2021.105234>
14. Ayipo, Y. O., Yahaya, S. N., Babamale, H. F., **Ahmad, I.**, Patel, H., & Mordi, M. N. (2021).  $\beta$ -Carboline alkaloids induce structural plasticity and inhibition of SARS-CoV-2 nsp3 macrodomain more potently than remdesivir metabolite GS-441524: computational approach. *Turkish journal of biology Turk biyoloji dergisi*, 45(4), 503–517.

<https://doi.org/10.3906/biy-2106-64>

15. Malani, A., Makwana, A., Monapara, J., **Ahmad, I.**, Patel, H., & Desai, N. (2021). Synthesis, molecular docking, DFT study, and in vitro antimicrobial activity of some 4-(biphenyl-4-yl)-1,4-dihydropyridine and 4-(biphenyl-4-yl) pyridine derivatives. *Journal of biochemical and molecular toxicology*, e22903. <https://doi.org/10.1002/jbt.22903>
16. Lee, H. Y., Cho, D. Y., **Ahmad, I.**, Patel, H. M., Kim, M. J., Jung, J. G., Jeong, E. H., Haque, M. A., & Cho, K. M. (2021). Mining of a novel esterase (est3S) gene from a cow rumen metagenomic library with organosphosphorus insecticides degrading capability: Catalytic insights by site directed mutations, docking, and molecular dynamic simulations. *International journal of biological macromolecules*, 190, 441–455. Advance online publication. <https://doi.org/10.1016/j.ijbiomac.2021.08.224>
17. Zrieq, R., **Ahmad, I.**, Snoussi, M., Noumi, E., Iriti, M., Algahtani, F. D., Patel, H., Saeed, M., Tasleem, M., Sulaiman, S., Aouadi, K., & Kadri, A. (2021). Tomatidine and Patchouli Alcohol as Inhibitors of SARS-CoV-2 Enzymes (3CLpro, PLpro and NSP15) by Molecular Docking and Molecular Dynamics Simulations. *International journal of molecular sciences*, 22(19), 10693. <https://doi.org/10.3390/ijms221910693>
18. Pawara, R., **Ahmad, I.**, Surana, S., & Patel, H. (2021). Computational identification of 2,4-disubstituted amino-pyrimidines as L858R/T790M-EGFR double mutant inhibitors using pharmacophore mapping, molecular docking, binding free energy calculation, DFT study and molecular dynamic simulation. *In silico pharmacology*, 9(1), 54. <https://doi.org/10.1007/s40203-021-00113-x>
19. **Ahmad, I.**, Pawara, R., Surana, S., & Patel, H. (2021). The Repurposed ACE2 Inhibitors: SARS-CoV-2 Entry Blockers of Covid-19. *Topics in current chemistry (Cham)*, 379(6), 40. <https://doi.org/10.1007/s41061-021-00353-7>
20. Ghosh, S., Das, S., **Ahmad, I.**, & Patel, H. (2021). In silico validation of anti-viral drugs obtained from marine sources as a potential target against SARS-CoV-2 Mpro. *Journal of the Indian Chemical Society*, 98(12), 100272. <https://doi.org/10.1016/j.jics.2021.100272>
21. I. Ahmad, S.R. Akand, M. Shaikh et al., Synthesis, molecular modelling study of the methaqualone analogues as anti-convulsant agent with improved cognition activity and minimized neurotoxicity, *Journal of Molecular Structure*, <https://doi.org/10.1016/j.molstruc.2021.131972>
22. Desai, N. C., Maheta, A. S., Jethawa, A. M., Pandit, U. P., **Ahmad, I.**, & Patel, H. (2022). Zeolite (Y-H)-based green synthesis, antimicrobial activity, and molecular docking studies of imidazole bearing oxydibenzene hybrid molecules. *Journal of Heterocyclic Chemistry*, 59(5), 879-889.
23. Pawara, R., **Ahmad, I.**, Nayak, D., Belamkar, S., Surana, S., Kundu, C. N., ... & Patel, H. (2021). Design and Synthesis of the Novel, Selective WZ4002 analogue as EGFR-L858R/T790M Tyrosine Kinase Inhibitors for Targeted Drug Therapy in Non-Small-Cell Lung Cancer (NSCLC). *Journal of Molecular Structure* 1254 (2022) 132313

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25. Acar Çevik, U., Celik, I., Işık, A., **Ahmad, I.**, Patel, H., Özkay, Y., & Kaplancıklı, Z. A. (2022). Design, synthesis, molecular modeling, DFT, ADME and biological evaluation studies of some new 1,3,4-oxadiazole linked benzimidazoles as anticancer agents and aromatase inhibitors. *Journal of biomolecular structure & dynamics*, 1–15. Advance online publication. <https://doi.org/10.1080/07391102.2022.2025906>
26. Boulaamane, Y., **Ahmad, I.**, Patel, H., Das, N., Britel, M. R., & Maurady, A. (2022). Structural exploration of selected C6 and C7-substituted coumarin isomers as selective MAO-B inhibitors. *Journal of Biomolecular Structure and Dynamics*, 1-15. <https://doi.org/10.1080/07391102.2022.2033643>
27. Cheke, R. S., Patil, V. M., Firke, S. D., Ambhore, J. P., **Ahmad, I.**, Patel, H. M., Shinde, S. D., Pasupuleti, V. R., Hassan, M. I., Adnan, M., Kadri, A., & Snoussi, M. (2022, February 22). Therapeutic Outcomes of Isatin and Its Derivatives against Multiple Diseases: Recent Developments in Drug Discovery. *Pharmaceuticals*, 15(3), 272. <https://doi.org/10.3390/ph15030272>
28. Girase, R., **Ahmad, I.**, Pawara, R., & Patel, H. (2022). Optimizing cardio, hepato and phospholipidosis toxicity of the Bedaquiline by chemoinformatics and molecular modelling approach. *SAR and QSAR in environmental research*, 1–21. Advance online publication. <https://doi.org/10.1080/1062936X.2022.2041724>
29. Osmaniye, D., Karaca, Ş., Kurban, B., Baysal, M., **Ahmad, I.**, Patel, H., Özkay, Y., & Asım Kaplancıklı, Z. (2022). Design, synthesis, molecular docking and molecular dynamics studies of novel triazolothiadiazine derivatives containing furan or thiophene rings as anticancer agents. *Bioorganic chemistry*, 122, 105709. Advance online publication. <https://doi.org/10.1016/j.bioorg.2022.105709>
30. Bharadwaj, K. K., **Ahmad, I.**, Pati, S., Ghosh, A., Sarkar, T., Rabha, B., Patel, H., Baishya, D., Edinur, H. A., Abdul Kari, Z., Ahmad Mohd Zain, M. R., & Wan Rosli, W. I. (2022). Potent Bioactive Compounds From Seaweed Waste to Combat Cancer Through Bioinformatics Investigation. *Frontiers in nutrition*, 9, 889276. <https://doi.org/10.3389/fnut.2022.889276>
31. Cheke, R. S., Patil, V. M., Firke, S. D., Ambhore, J. P., **Ahmad, I.**, Patel, H. M., Shinde, S. D., Pasupuleti, V. R., Hassan, M. I., Adnan, M., Kadri, A., & Snoussi, M & Deshmukh, P. K. (2022). Molecular Insights into Coumarin Analogues as Antimicrobial Agents: Recent Developments in Drug Discovery. *Antibiotics (Basel, Switzerland)*, 11(5), 566. <https://doi.org/10.3390/antibiotics11050566>
32. Kumar, P., Pandey, R., Dubey, I., **Ahmad, I.**, Mahapatra, D. K., & Patel, H. (2022,

- August). In silico Study of Some Dexamethasone Analogs and Derivatives against SARs-CoV-2 Target: A Cost-effective Alternative to Remdesivir for Various COVID Phases. *Current Chinese Science*, 2(4), 294–309. <https://doi.org/10.2174/2210298102666220404102217>
- 33 Radwan HA, **Ahmad, I**, Othman IM, Gad-Elkareem MA, Patel H, Aouadi K, Snoussi M, Kadri A. Design, synthesis, in vitro anticancer and antimicrobial evaluation, SAR analysis, molecular docking and dynamic simulation of new pyrazoles, triazoles and pyridazines based isoxazole. *Journal of Molecular Structure*. 2022 May 16:133312. <https://doi.org/10.1016/j.molstruc.2022.133312>
- 34 **Ahmad I**, Pawara RH, Girase RT, Pathan AY, Jagatap VR, Desai N, Ayipo YO, Surana SJ, Patel H. Synthesis, Molecular Modeling Study, and Quantum-Chemical-Based Investigations of Isoindoline-1,3-diones as Antimycobacterial Agents. *ACS Omega*. 2022 Jun 10;7(25):21820-21844. doi: 10.1021/acsomega.2c01981. PMID: 35785272; PMCID: PMC9244950.
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- 36 Chaudhari B, Patel H, Thakar S, **Ahmad I**, Bansode D. Optimizing the Sunitinib for cardio-toxicity and thyro-toxicity by scaffold hopping approach. *In Silico Pharmacol*. 2022 Jul 2;10(1):10. doi: 10.1007/s40203-022-00125-1. PMID: 35791431; PMCID: PMC9250587.
- 37 Farhan MM, Guma MA, Rabeea MA, **Ahmad I**, Patel H. Synthesizes, Characterization, Molecular docking and in vitro Bioactivity study of new compounds containing Triple Beta Lactam Rings. *Journal of Molecular Structure*. 2022 Jul 23:133781. <https://doi.org/10.1016/j.molstruc.2022.133781>
- 38 Ayipo, Y. O., Alananzeh, W. A., **Ahmad, I**, Patel, H., & Mordi, M. N. (2022, July 26). Structural modelling and in silico pharmacology of  $\beta$ -carboline alkaloids as potent 5-HT<sub>1A</sub> receptor antagonists and reuptake inhibitors. *Journal of Biomolecular Structure and Dynamics*, 1–17. <https://doi.org/10.1080/07391102.2022.2104376>
- 39 **I. Ahmad**, R. Pawara & H. Patel In silico toxicity investigation of Methaqualone's conjunctival, retinal, and gastrointestinal hemorrhage by molecular modelling approach <https://doi.org/10.1080/08927022.2022.2113412>
- 40 Pathan, A., **Ahmad, I**, Girase, R., Jagatap, V., & Patel, H. (2022, August 23). A Laboratory Accident of Acryloyl Chloride, Its Consequences, Treatment, and Safety Measures: An Arduous Lesson to All Researchers. *ACS Chemical Health & Safety*, 29(5), 405–420. <https://doi.org/10.1021/acs.chas.2c00036>
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- [Snoussi, M.; \*\*Ahmad, I.\*\*; Aljohani, A.M.A.; Patel, H.; Abdulhakeem, M.A.; Alhazmi, Y.S.; Tepe, B.; Adnan, M.; Siddiqui, A.J.; Sarikurkcu, C.; Riadh, B.; Feo, V.D.; Alreshidi, M.; Noumi, E. Phytochemical Analysis, Antioxidant, and Antimicrobial Activities of Ducrosia flabellifolia: A Combined Experimental and Computational Approaches. \*Antioxidants\* 2022, 11, 2174. <https://doi.org/10.3390/antiox11112174>](https://doi.org/10.3390/antiox11112174)
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- [Puri, S., \*\*Ahmad, I.\*\*, Patel, H., Kumar, K., & Juvale, K. \(2023, February\). Evaluation of oxindole derivatives as a potential anticancer agent against breast carcinoma cells: In vitro, in silico, and molecular docking study. \*Toxicology in Vitro\*, 86, 105517. <https://doi.org/10.1016/j.tiv.2022.105517>](https://doi.org/10.1016/j.tiv.2022.105517)
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### Books and Book Chapter Published

Title	Publisher	year	ISBN/ISSN No.
Herbal Cosmetics-III, A Practical Lab Manual	Unnati Publications	2021	941-927-20-0941-0
Natural Products as Enzyme Inhibitors: An Industrial Perspective	Springer Nature	2022	978-981-19-0932-0 (eBook)

### Conference /Workshop/FDP/STTP Attended

#### National: 10

1. Attended DST funded Synergistic training program utilizing the scientific and technological infrastructure (STUTI) programme and work as Demonstrator in Computer Aided Drug Designing (CADD), from 20<sup>th</sup>-26<sup>th</sup> June 2022.
2. Attended Five Days webinar series Dive into The World of Drug Discovery, Organized by Schrödinger and Biotechnika Info Labs Pvt. Ltd, from 5<sup>th</sup> to 09<sup>th</sup> August 2021.
3. Attended AICTE Delhi sponsored One-Week Online STTP “Scientific Research Paper, Patents and Research Proposal Writing for Grants and an Ethics” organized by R. C. Patel Institute of Pharmaceutical Education and Research, Shirpur from 5<sup>th</sup> to 10<sup>th</sup> June 2021.
4. Attended International virtual conference on Computer-Aided Drug Design organized by Department of Pharmacy, BITS Pilani, Pilani campus from October 30 to 31, 2020.

5. Attended One Week National Online Faculty Development Program on ICT Tools for Effective Teaching Learning, organized by School of Mathematical Sciences, Swami Ramanand Teerth Marathwada University, Nanded, from 11<sup>th</sup> to 16<sup>th</sup> May 2020.
6. Attended five-day e-faculty development program on “building research and innovative culture among pharmacy teachers” organized by D.Y. Patil Institute of Pharmaceutical Education and Research, Pimpri Pune in association with association of pharmacy teachers of India, from 18<sup>th</sup> to 22<sup>nd</sup> may 2020,
7. Attended one-day National Level Seminar on “Innovative concepts and Methodologies in pharmaceutical Research” Organized by HRPIPER Shirpur, Dhule, held on 10<sup>th</sup> March 2018.
8. Poster Presented in Pharmeet 2016 “Emerging Prospects in Pharmaceutical industry” organized by MITCON Pune on 06<sup>th</sup> February 2016.
9. Attended one-day National conference on “Structure Interpretation of Organic Compound” Organized by RCPIPER Shirpur, Dhule, on 24<sup>th</sup> September 2016.
10. Attended state level seminar on “Green chemistry and chemical waste management” Sponsored by Savitribai Phule University, Pune, on 25<sup>th</sup> January 2016.

**International:** NIL

### Professional Membership

Life time Member of Maharashtra State Pharmacy Council (**Registration Number: 194287**)