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- Research area: Medicinal & Organic Chemistry – Anticancer, Anti- HIV, Anticonvulsant, Antitubercular, Antimalarial, Drug Design, Molecular Docking & AI in Drug Delivery
- 152 Publications, 2 Patents, 4 Books & 2 Books chapters
- Advisor: 1 Ph.D. & 45 Master degree



Publications (current):

1. Azam, F.; Khan, A.; **Ahsan, M.J.** Targeting tubulin protein by novel 3,5-disubstituted-1,2,4-triazole analogues as anticancer agents: Design, synthesis, in-vitro, and in-silico studies. *J. Mol. Struct.*, **2025**, 1331, 141574.
2. Sharma, R.; Salahuddin; Mazumder, A.; Kumar, R.; Chauhan, A.; **Ahsan, M.J.**; Shahar Yar, M.; Maqsood, R.; Singh, S. Pyrazoline Derivatives: Exploring the Synthesis and Development of New Ligands for Anti-Cancer Therapy. *Med Chem.*, **2025**, 21, 264-293. <http://dx.doi.org/10.2174/0115734064339011241129075522>
3. **Ahsan, M.J.***; Kumar, V.; Ali, A.; Ali, A.; Yusuf, M.; Ahamed, I.; Patel, H.; Salahuddin, Ahsan, M.F. Design, Synthesis, And Biological Evaluations of Newer 5-Aryl-N-(Naphthalen-2-yl)-1,3,4-Oxadiazol-2-Amines: An Insight into Experimental and In-Silico Investigations. *Fut. Med. Chem.*, **2025**. <https://doi.org/10.1080/17568919.2025.2504335>
4. Mangal, S.; Salahuddin, Mazumdar, A.; Kumar, R.; Rani, S.; **Ahsan, M.J.**; ShaharYar, M. Significant Advances in Catalytic Strategies for the Synthesis of Trisubstituted Imidazoles: A Review. *Synth. Comm.*, **2025**. <https://doi.org/10.1080/00397911.2025.2505901>
5. Sharma, A.S.; Salahuddin; Rana K.; Debnath, A.; Mazumder, A.; Kumar, R.; **Ahsan, M.J.**; Shahar Yar, M.; Tyagi, P.K. Singh, S. Synthesis, anticonvulsant potential, and molecular docking studies of Schiff bases bearing 2',6-dichloro-2,3'-biquinoline. *Indian J. Het. Chem.*, **2022**, 32, 209-216.
6. Kumar, D.; Salahuddin; Mazumder, A.; Kumar, R.; **Ahsan, M.J.**; ShaharYar, M.; Abbussalam; Tyagi, P.K.; Chaitanya, M.V.N.L. Pharmacological Evaluation of Bioisosterically Replaced and Triazole-Tethered Derivatives for Anticancer Therapy. *Med. Chem.*, **2025**, 21, 264-293.
7. Afzal, O.; **Ahsan, M.J.** An Efficient Synthesis of 1-(1,3-Dioxoisooindolin-2-yl)-3-aryl Urea Analogs as Anticancer and Antioxidant Agents: An Insight into Experimental and In Silico Studies. *Molecules* **2024**, 29, 67.
8. Ahsan, M.F.*; Yusuf, M.; Ansari, M.Y.; Sahoo, G.C.; Salahuddin, Murthy, N.M.; **Ahsan, M.J.***; Riadi, Y. An Efficient Synthesis of Curcumin Pyrazole Analogues and their Biological Activities. *Org. Prep. Proce. Int.*, **2024**, 56, 467-475.

9. Chauhan, A.; Salahuddin; Mazumder, A.; Kumar, R.; **Ahsan, M.J.**; Shaharyar, M.; Maqsood, R.; Singh, S.K. Targeted Development of Pyrazoline Derivatives for Neurological Disorders: A Review. *ChemistrySelect*, **2024**, 9, e202400738.
10. **Ahsan, M.J.***; Sarwar, A.; Ali, A.; Ali, A.; Ahmad, M.D.; Hedaytullah, M.; Salahuddin, Ahsan, M.F.; Riadi, Y. An Efficient Synthesis of Novel Semicarbazones and Their Biological Activities. *Org. Prep. Proce. Int.*, **2024**, 56, 597-605.
11. **Ahsan, M.J.***; Khandelwal, K.; Ali, A.; Ali, A.; Riadi, Y.; Geesi, M.H.; Aldakhil, T.; Ahsan, M.F.; Tahir, A.; Azam, F.; Salahuddin. Solvent-free Synthesis, Anticancer Activity and In-Silico Studies of 7-Hydroxy-4-methylquinolin-2(1H)-one Analogues. *J. Mol. Struct.*, **2024**, 1313, 138654.
12. Mohamed, M.A.; Ali, A.; Ali, A.; Afzal, O.; Ahsan, M.F.; Mubarak, M.A.; Alossaimi, M.A.; Altamimi, A.S.A.; Salahuddin; **Ahsan, M.J.*** Targeting EGFR by Newer 1-(3,5-Bis((E)-4-hydroxy-3-methoxystyryl)-1H-pyrazol-1-yl)-2-((substituted phenyl)amino)ethan-1-one Analogues for the Treatment of Cancer: Synthesis, In-vitro and In-silico Studies. *J. Mol. Struct.*, **2024**, 1315, 138826.

Patents:

1. Chakraborty, T.; Saini, V.; Kaur, M.; Garg, V.; Kaushik, V.; Naik, K.K.; Kumar, M.; **Ahsan, M.J.**; Jain, S.; Sharma, V.; Pushkarna, N. Novel simultaneous estimation methods of three combined pure drugs and its novel formulation by UV spectrophotometer (Patent Application No. 201611032463)
2. Salahuddin; Yar, M.S.; Rana, K.; Mazumdar, A.; Kumar, R.; Verma, S.; **Ahsan, M.J.**; Yadav, S.K.; Yadav, S. Solvent free synthesis of benzimidazole derivatives" (Patent Application No. 202311007058 A)

Research Projects (Completed):

1. Title: **Targeting tubulin protein by novel 3,5-Disubstituted-1,2,4-Triazole Analogues for the treatment of cancer: Design, synthesis, in-vitro, and in-silico studies;** Co-investigator M. Jawed Ahsan; Abstract: This article discusses the design, synthesis, characterization, cytotoxic activity against cancer cells, and computational studies of four novel *N*-aryl-5-phenyl-4*H*-1,2,4-triazol-3-amines (**4a-d**). Cost: 15.84 Lakhs
Publication: <https://doi.org/10.1016/j.molstruc.2025.141574>
2. Title: **In-silico screening of carbonic anhydrase inhibitors for the treatment of oxidative stress at high altitude: 3D-QSAR, Pharmacophore modelling, virtual screening and molecular docking studies**
Cost: 44 Lakhs
Publications: <https://doi.org/10.3390/molecules27010309>
<https://doi.org/10.3390/cimb44030068>
<https://doi.org/10.3390/ijms23095054>
3. Title: **Solvent-free Synthesis of 1-(1, 3-Dioxoisoindolin-2-yl)-3-aryl Urea Analogs as Anticancer Agents: An Insight into Experimental and In Silico Studies;** Co-Investigator – M. Jawed Ahsan; Objectives: *a) To design, synthesis and anticancer activity of new 1-(1, 3-Dioxoisoindolin-2-yl)-3-aryl Urea Analogs, b) To discover potent, selective and orally efficacious EGFR inhibitor, c) To establish pharmacophore group responsible*

for anti-EGFR & anticancer activities in proposed analogues, d) Carry out molecular docking simulation of substituted 1-(1, 3-Dioxoisindolin-2-yl)-3-aryl urea analogs at EGFR binding site to establish binding mode, e) To evaluate anticancer activity of synthesized compounds against various cancer cell lines.

Publications: <https://doi.org/10.3390/molecules29010067>

Research Projects (Undergoing):

1. Title: **Pharmacophore Based Designing and Synthesis of Newer Oxadiazoles: Search for Tubulin Antagonist as Anticancer Agents;** Principal Investigator – M. Jawed Ahsan; **Objectives:** *a) To design, synthesis and anticancer activity of new oxadiazole analogues, b) To discover potent, selective and orally efficacious tubulin inhibitor, c) To establish pharmacophore group responsible for anti-tubulin & anticancer activities in proposed analogues, d) Carry out molecular docking simulation of substituted oxadiazoles at tubulin-colchicine binding site to establish binding mode, e) To measure the binding affinity of synthesized compounds to the tubulin-colchicine binding site, f) To evaluate anticancer activity of synthesized compounds against various cancer cell lines.*

Books &/or Book Chapters:

1. Design, Synthesis and Anti-HIV Activity of Curcumin Analogues. **Ahsan, M.J.** and Sharma, S. Ed. Irina Rusu, **2015**; Lambert Academic Publishing, Germany ISBN: 978-3-659-75001-4.
2. Molecular Properties Prediction and Synthesis of Oxadiazole Analogues As Antimicrobial Agent. Sharma, R.; Sharma, P.; **Ahsan, M.J.** Ed. Irina Rusu, **2015**; Lambert Academic Publishing, Germany ISBN: 978-3-659-75863-8
3. Synthesis and Characterization of Nateglinide Derivatives. Sharma, R and **Ahsan, M.J.** Ed. Irina Rusu, **2015**; Lambert Academic Publishing, Germany ISBN: 978-3-659-76920-7
4. Development of New Process for the Synthesis of Intermediates of Etoricoxib, Pioglitazone and Niacin. Kumawat, V.; **Ahsan, M.J.** 2020; Ed., Veronica Virlan, Lambert Academic Publishing, Germany ISBN: 978-620-0-56584-6
5. Translational Research and Clinical Advancements with Nutraceutical Supplements, (*book chapter - “Synbiotics in Human Health: Biology to Drug Delivery”*), Agrawal, M., Sharma, P., Garg, S., Bhatia, S., Laxmikant, Sharma, B., Dwivedi, A., Goyal, P.K., Chauhan, A., **Ahsan, M.J.**, Chaudhary, H., pp 647–662, *Online*, 30 March **2024**.
https://doi.org/10.1007/978-981-99-5575-6_33
6. Antitubercular Agents and Tubercular Vaccines in Clinical Trials, (*book chapter – “Frontiers in Anti-Infective Drug Discovery”*), **Ahsan, M.J.**, Vol. 6, pp. 282-334, Bentham Science Publishers. <https://www.eurekaselect.com/chapter/10847>

Posters, Presentations, & Conferences (recent):

1. Synthesis of Pyrazole Curcumin Analogues: A Productivity-Boosting Catalytic Approach with In-vitro and In-Silico Studies, Ahsan, M.J.; Yusuf, M.; Ansari, M.Y.; Sahoo, G.C. **“International Conference on Novel Paradigms in Pharmaceutical Sciences”**, OP-37, pp. 44, 9-10 March 2024, Integral University, Lucknow, India.