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PROFILE

- **PhD & MSc in Bioinformatics** with Post Graduate Diploma in NanoBiotechnology & Food Processing & Preservation
- **Expert in Cancer Bioinformatics:** Over 17 years of dedicated research & academic experience in Cancer Bioinformatics, specializing in the simulation of cancer pathways and in silico chemoprevention studies with both natural and synthetic compounds.
- **Innovative Algorithm Development:** Proficient in developing and applying genetic algorithms and artificial neural networks to enhance predictive modeling in molecular biology and bioinformatics.
- **Completed Research Projects:** Successfully completed **two Young Scientist projects funded by the Council of Science and Technology (CST), Uttar Pradesh, and the Indian Council of Medical Research (ICMR)**, contributing to advancements in cancer bioinformatics.
- **Research Publication and Presentation:** Proven track record of publishing **more than 100 papers** in high-impact journals and presenting findings at international conferences, fostering collaboration and establishing a robust academic network.
- **Mentorship and Teaching Excellence:** **Honorary faculty member and active mentor at Novel Global Community Educational Foundation (NGCEF), Australia**, guiding B.Tech and M.Tech students in bioinformatics and biotechnology.
- **Quality Assurance and Accreditation Leadership:** **NAAC Criteria III Grants/Projects In-Charge at central level & NAAC Criteria III In-Charge** at departmental, overseeing quality assurance processes and contributing to academic program accreditation.
- **Committee Involvement and Academic Governance:** **Board of Studies Coordinator, Member of the Faculty Board, and Academic Council** at Integral University, actively participating in governance and curriculum development initiatives.
- **Program Coordinator** for M. Tech Bioinformatics program.
- **Course Coordinator** for M. Tech Biotechnology programs.
- Member of the University Examination Committee, Flying Squads, ACS, and Core Committees and Member of University & Department Quality Assurance Cell.
- Member of the Journal Club in the Department of Bioengineering.

RESEARCH INTEREST:

- Cancer Bioinformatics and Simulation of Cancer Pathways
- Computer aided Drug Designing: Molecular Docking and QSAR studies, MD simulations.
- Gene Expression Analysis
- Algorithms for Molecular Biology: Genetic Algorithms and Artificial Neural networks.

SUMMARY OF RESEARCH ACCOMPLISHMENT:

- **Young Scientist Project:** Awarded a prestigious project titled “Dynamic Structure-Based Pharmacophore Model Development and Role of Dietary Phytochemicals: A Crosstalk and Effective Addition in Anti-Angiogenic Lead Discovery” by the Uttar Pradesh Council of Science and Technology (UPCST), Government of Uttar Pradesh.
- **ICMR-SRF Project:** Research project on “Structure-Based Virtual Screening, Molecular Docking, and Simulation Studies of Quinazoline Derivatives for Their Anti-EGFR Activity Inhibiting Tumor Angiogenesis” (Project ID: 2021-13015) in the Department of Bioengineering.
- **Research Publications:** Authored over 100 research papers and 5 book chapters in esteemed peer-reviewed national and international journals.
- **Committee Involvement:** Active member of the Research Committee at **Novel Global Community Educational Foundation (NGCEF), Australia.**
- **Editorial Roles:** Serve as an editorial member for 3 journals and as a Guest editor for 5 reputed journals.
- **Intellectual Property:** Hold three patents related to advancements in bioinformatics and drug design.
- **Ph.D. Supervision:** Guided seven Ph.D. candidates through their Doctoral studies.
- **Thesis Evaluation:** Evaluated Ph.D. thesis for CSIR Labs, contributing to academic rigor and quality assurance.
- **Conference Contributions:** Published over 100 abstracts in the proceedings of various national and international conferences and seminars.
- **Peer Review Service:** Invited reviewer for over 40 peer-reviewed national and international journals, enhancing the quality of scientific publications.

PROFESSIONAL MEMBERSHIP:

- Member of European Association for Cancer Research (EACR), Nottingham.
- Member of International Association of Engineers, Hong Kong.
- Senior Member of International Society for Research and Development (ISRDR), London.

COURSE TAUGHT:

B.Tech

- Advanced Bioinformatics
- Bioinformatics Project

M.Tech

- Bioinformatics, Genomics & Proteomics

- Computer Aided Drug Design
- Chemoinformatics & Pharmacogenomics
- Algorithms in Molecular Biology

B.Sc.

- Computational Life Sciences & Bioinformatics

M.Sc.

- Bioinformatics and Biostatistics
- Bioinformatics & Applied Statistics

ADMINISTRATIVE/DEPARTMENTAL RESPONSIBILITY

- **Quality Assurance Leadership:**
 - NAAC Criteria III In-Charge (Departmental).
 - NAAC Criteria III Project/Grant In-Charge (Central).
- **Committee Membership:**
 - Member of Flying Squads and Assistant Centre Superintendent (ACS).
 - Lawn Committee (Central Convocation).
 - Member of the University Examination Committee, Core Committees, and University & Department Quality Assurance Cell.
 - Member of the Journal Club in the Department of Bioengineering.
- **Board of Studies Coordinator**
- **Governance Involvement:**
 - Member of the FAC, Faculty Board, and Academic Council at Integral University.
 - Actively participate in governance and curriculum development initiatives.
- **Program Coordination:**
 - Program Coordinator for M.Tech Bioinformatics.
 - Course Coordinator for M.Tech Biotechnology programs.
- **Workshop and Conference Organization:**
 - Organized workshops and conferences as convener and co-convener to provide a platform for the exchange of novel ideas and promote collaborative research.

STUDENTS SUPERVISION

PHD AWARDED

- Neha Sharma (M Tech Biotechnology, DST INSPIRE Fellow, Government of India)
- Surabhi Yadav (M Sc. Biotechnology, JRF, SGPGI, Lucknow)
- Mala Sharma (M Sc. Bioinformatics, Integral University)
- Swati Gautam (M Sc. Biochemistry, ICMR- JRF, KGMU, Lucknow)
- Alok Singh (Research Fellow, Era Medical College, Lucknow)
- Altaf Ahmad Shah (ICMR- SRF, Integral University)
- Co-Supervision of Syed Sayeed Ahmad (M Tech Biotechnology, Integral University).

- Co-Supervisor of Shalini Maurya (DBT-JRF, Integral University).

PhD REGISTERED

- Ruqqaiya Quddus (M Tech Bioinformatics)
- Fariya Atif (M Tech Biotechnology)
- Amna Tamimi (M Tech Bioinformatics)
- Mantasha Khan (M Tech Bioinformatics)
- Co-Supervisor of Suhail Ahmad (M Tech Biotechnology)

Post Graduate Supervision

- **Hina Khatoon:** Identification of Bioagents of *Andrographis paniculata* (Kalmegh) and their antimicrobial effect.
- **Naziya Farheen:** Evaluation of terpenoids as dipeptidyl 4 inhibitors: Molecular docking study.
- **Anubhav:** Exploring the anti-angiogenesis potential of brassicanal B and its derivatives targeting Hsp90 protein: An in-silico perspective.
- **Swaraj Dubey:** A neuroinformatics approach towards screening and elucidation of selected alkaloids for their anti-Alzheimer potential targeting AChE protein.
- **Mohammad Armoghan:** Virtual screening and molecular docking studies of natural inhibitors against cytochrome P450 1A2.
- **Shrinarayan Tripathi:** Efficacy of natural inhibitors against cytochrome P450 1A2: An in-silico approach to combat mammary cancer.
- **Farman Khan:** Elucidation of the effect of selected natural inhibitors against cytochrome P450 1A2: An in-silico approach to combat mammary cancer.
- **Vertika Singh:** Virtual screening of plant-derived natural compounds as inhibitors of cytochrome P450 1A1.
- **Mohd Rahil:** Deciphering the antiangiogenic potential of brassicanal B and its derivatives targeting Hsp90 protein: A novel in-silico multipathway targeted move to refrain angiogenic phenomena.
- **Roohi Kumari Parsad:** Efficacy of natural inhibitors against cytochrome P450 1A2: An in-silico approach to combat mammary cancer.
- **Sonee Rajpoot:** Insights from the docking simulation of plant-derived natural compounds as cancer prevention through inhibiting hypoxia-inducible factor 1 alpha.
- **Mohd Shamshad Khan:** Virtual screening and in-silico elucidation of the anti-Alzheimer's potential of selected alkaloids targeting AChE protein: A neuroinformatics study.
- **Farrukh Naz:** Network construction of metformin, afrezza, and tanzeum drug pathways using Cytoscape.
- **Anjali Tiwari:** Virtual screening of polyphenols for their anti-Parkinson's disease potential inhibiting alpha-synuclein.
- **Isma Rafee:** Screening and elucidation of the anti-Alzheimer potential of selected alkaloids targeting AChE protein: A neuroinformatics study.
- **Sana Maryam Atif:** Screening of selected alkaloids as potent dual inhibitory agents against Alzheimer's disease targeting BACE-1 protein and β -Amyloid aggregation: A neuroinformatics study.
- **Nadeem Khan:** Screening of marine compounds for their anti-HPV potential resisting cervical cancer by targeting critical E6 protein involved in the degradation of p53: A computational case study.

- **Shaheen Khan:** Deciphering the antiangiogenic potential of brassicanal B and its derivatives targeting Hsp90 protein: A novel in-silico multipathway targeted move to refrain angiogenic phenomena.

PUBLISHED/GRANT PATENTS

- ARTIFICIAL INTELLIGENCE BASED SMART SYSTEM FOR HEART SOUND DETECTION AND CLASSIFICATION USING SIGNAL PROCESSING AND MACHINE LEARNING ALGORITHMS TO AVOID HEART ATTACK AND OTHER HEART DISEASES (Indian Patent) 06/10/2023
- AI BASED SAFE HEALTHCARE SYSTEM FOR FERTILITY PRESERVATION FOR YOUNG WOMAN WITH BREAST CANCER USING CLOUD AND MACHINE LEARNING ALGORITHMS (Indian Patent) 13/10/2023
- ARTIFICIAL INTELLIGENCE BASED (BP) BLOOD-PRESSURE DROPPING SYSTEM FOR AVOIDANCE OF CARDIOVASCULAR DISEASE USING DATA MINING AND MACHINE LEARNING TECHNIQUES FOR HEALTH CARE MANAGEMENT (INDIAN PATENT) 01/09/2023

PUBLISHED/ACCEPTED SCI/SCOPUS RESEARCH PAPERS

- Akhtar, S.; Al-Sagair, O.A. and Arif, J.M. Novel aglycones of steroidal glycoalkaloids as potent tyrosine kinase inhibitors: Role in VEGF and EGF receptors targeted angiogenesis. (2011), *Letters in Drug Design & Discovery*, 8(3), pp-205-215. (Impact Factor = 1.099)
- Khan, M.S.; Akhtar, S.; Arif, J.M., Al-Sagair, O. Protective effect of dietary tocotrienols against infection and inflammation-induced hyperlipidemia: An in vivo and in silico study. (2011), *Phytotherapy Research*, 25, pp-1586-1595. (Impact Factor = 6.388)
- Khan, M.K.A; Akhtar, S. and Arif, J.M. Homology Modeling of CYP1A1, CYP1B1 and its Subsequent Molecular Docking Studies with Resveratrol and its Analogues using AutoDock Tools 4.0, (2011), *Biochem. Cell. Arch.* 11(1).
- Khan, M.K.A; Akhtar, S., Siddiqui, M.H., Al-Sagair, O. and Arif, J.M., Insilico Elucidation and Validation of Metabolic activation/detoxification process of dibenzo (a, l) pyrene and its metabolites using AutoDock Tools 4.0., (2011), *J. Chem. Pharm. Res.*, 3(1), pp-756-763.
- Arif, J.M.; Siddiqui, M.H.; Akhtar, S. and Al-Sagair, O. Exploitation of in silico potential in prediction, validation and elucidation of mechanism of anti-angiogenesis by novel compounds: Comparative correlation between wet lab and in silico data. (2013) *Int J Bioinform Res Appl.*, 9(4), 336-48. doi: 10.1504/IJBRA.2013.054697. PMID: 23797993.

- Khan, M.S.; Akhtar, S.; Siddiqui, S.A.; Siddiqui, M.S.; Srinivasan, K.V. and Arif, J.M. Design, Synthesis and Evaluation of Unique 2,4,5-triaryl Imidazole Derivatives as Novel Potent Aspartic Protease Inhibitors (2012), *Medicinal Chemistry* 8(3), pp-428-35. (Impact Factor = 2.329)
- Gupta, C.L.; Akhtar, S.; Bajpai, P.; Kandpala, K.N.; Desai, G.S. and Tiwari, A.K. Computational Modeling and Validation studies of 3-D structure of Neuraminidase protein of H1N1 Influenza A virus and Subsequent Insilico Elucidation of Piceid analogues as its Potent Inhibitors (2013), *EXCLI*, 12, 215-25. (Impact Factor = 4.022)
- Srivasatva, R.; Akhtar, S.; Sharma, R. and Mishra, S. Identification of Ellagic acid analogues as potent inhibitor of protein Kinase CK2: A chemopreventive role in oral Cancer (2015), *Bioinformation*, 11(1), pp- 21-26. (PubMed Indexed)
- Al-Khodairy, F.M.; Khan, M.K.A.; Kunhi, M.; Pulicat, M.S.; Akhtar, S. and Arif, J.M. In Silico Prediction of Mechanism of Erysolin-induced Apoptosis in Human Breast Cancer Cell Lines, (2013), *Am J Bioinfo Res*, 3(3), pp- 62-71.
- Shaikh S, Ahmad SS, Ansari MA, Shakil S, Rizvi Smd, Shakil SS, Tabrez S, Akhtar S, Kamal MA and Damanhoury GA. Prediction of Comparative Inhibition Efficiencies for a Novel Natural Ligand, Galangin Against Human Brain Acetylcholinesterase, Butyrylcholinesterase and 5-Lipoxygenase: A Neuroinformatics Study. (2014), *CNS Neurol Disord Drug Targets.*, 13(3), pp- 452-9. (Impact Factor = 2.824)
- Gupta C.L., Akhtar S. and Bajpai P. *IN SILICO* Protein Modeling: Possibilities And Limitations. (2014), *EXCLI*, 13, pp- 513-15. (Impact Factor = 4.022)
- Sayeed U, Wadhwa G, Khan M K A, Jamal Q M S, Akhtar S, Khan M S. An Immuno-informatics driven Epitope study from the molecular interaction of JEV non-structural (NS) proteins with Ribophorin (RPN). (2014) *Bioinformation*, 10(8), pp- 496-501. (PubMed Indexed)
- Gupta C.L., Akhtar S., Kumar N., Ali J., Pathak N., Bajpai P. In Silico Elucidation and Inhibition Studies of Selected Phytoligands against Mitogen Activated Protein Kinases of Protozoan Parasites. (2016) *Interdiscip Sci Comput Life Sci (Springer)* Mar, 8(1), pp- 41-52. (Impact Factor = 3.492)
[Awarded Second Best paper in the Journal for Year 2016 with 300\$ prize money]
- Sinha M., Khan M.K.A., Siddiqui M.H., Sayeed U., Wadhwa G. and Akhtar S.* Pharmacogenomics: A Step Ahead in Modern Day Drug Discovery (2014), *Int. J of Adv. in Eng. & Sci. Res.*, 1(8), pp 13-26.
- Khan M.K.A., Siddiqui M.H., Akhtar S., Ahmad K., Baig M.H. and Osama K. Screening of plant-derived natural compounds as potent chemotherapeutic agents against breast cancer: An *in silico* approach. (2015), *J. Chem. Pharm. Res.*, 7(1), pp-519-526.

- Gupta C.L., Akhtar S., Waye A., Pandey N.R., Pathak N., Bajpai P. Cross talk between Leishmania donovani CpG DNA and Toll-like receptor 9: An immunoinformatics approach. (2015), Biochem Biophys Res Commun.(BBRC), 459(3), pp- 424-9. (Impact Factor = 3.322).
- Gupta C.L., Akhtar S., Uzma A., Pathak N. and Bajpai P. Insilico analysis of human Toll-like receptor 7 ligand binding domain. (2016), Biotechnol Appl Biochem. 63(3):441-50 (Impact Factor = 2.724)
- Sayeed U., Jamal Q.M.S., Khan M.S., Wadhwa G., Siddiqui M.H. and Akhtar S. In silico Interaction Analysis of Intracranial Pressure Reducing Agent Mannitol and its Derivatives with Human Serum Albumin. (2015), Int. J of Scientific & Engineering Research, 6(4), 1688-92.
- Shahi N., Hasan A., Akhtar S., Siddiqui M .H., Sayeed U. and Khan M.K.A. Xylanase: A promising enzyme. (2016), J. Chem. Pharm. Res., 8(3), 334-339.
- Trivedi P., Hasan A., Akhtar S., Siddiqui M .H., Sayeed U. and Khan M.K.A. Role of microbes in degradation of synthetic plastics and manufacture of bioplastics. (2016), J. Chem. Pharm. Res., 8(3), 211-216.
- Alam A., Rizvi I.F., Sayeed U., Khan M.K.A., Akhtar S., Farooqui A. and Siddiqui M.H. Application of Nanotechnology in agriculture and food science. (2016), World J of Pharm Sci., 4(7), 45-54.
- Bishwas N., Sharma M., Hasan A., Akhtar S*, Sharma N. Improvement of rice crop by Marker-assisted Backcross method (2016), Int. Res. J of Engg & Tech. (IRJET)., 3(6), 1851-58.
- Bano N., Rizvi I.F., Sharma N., Siddiqui M.H., Khan M.K.A., Akhtar S*. Production of Bioactive Secondary Metabolites from Endophytic fungi (2016), Int. Res. J of Engg & Tech. (IRJET)., 3(6), 1859-66.
- Sarkar S., Osama K., Jamal Q.M.S, Kamal M.A., Sayeed U., Khan M.K.A., Siddiqui M.H., Akhtar S*, Advances and implications in nanotechnology for lung cancer management (2017), Current Drug Metabolism, 18(1), 30-38. (Impact Factor = 3.408)
- Sarkar A., Fatima J., Jamal Q.M.S., Sayeed U., Khan M.K.A., Akhtar S., Kamal M.A., Farooqui A., Siddiqui M.H., Nanoparticles as a Carrier System for Drug Delivery Across Blood Brain Barrier (2017), Current Drug Metabolism, 18(2):129-137 (Impact Factor = 3.408)
- Ahmad S.S., Akhtar S., Jamal Q.M.S., Rizvi S.M.D., Kamal M.A., Khan M.K.A., Siddiqui M.H. Multiple targets for management of Alzheimer's disease (2016), CNS & Neurological Disorders-Drug Targets, 15(10), 1279-1289. (Impact Factor = 2.824)

- Rehman A., Akhtar S., Siddiqui M.H., Sayeed U., Ahmad S.S., Arif J.M and Khan M.K.A. Identification of potential leads against 4-hydroxy-tetrahydrodipicolinate synthase from *Mycobacterium tuberculosis* (2016), *Bioinformation*, 12 (11), 400-07 (PubMed Indexed).
- Shakeel E., Arora D., Jamal Q.M., Akhtar S., Khan M.K.A., Kamal M.A., Siddiqui M.H., Lohani M. & Arif J.M. Marine drugs: A hidden wealth and a new epoch for cancer management. (2018), *Curr Drug Metab.* 19(6):523-543. (Impact Factor = 3.408)
- Bano T., Akhtar S., Siddiqui M.H., Arif J.M., Lohani M., Sayeed U. and Kalim M.K.A. Peptide Based Vaccine Design For Therapeutic Intervention. Against HTLV-I : A Computational Approach (2017)., *Biochem. Cell. Arch.* 17(2), 777-788.
- Gautam S., Jain A., Akhtar S., Priyadarshini A., Jaiswar S.P. Serum Vitamin D Level as a Risk Factor for Female Genital Tuberculosis (FGTB). (2017), *J Clin Diagn Res.*,11(9), 18-20.
- Yadav S, Akhtar S., Agarwal S.K., Majumdar G., Vimal S. Genetic Association of KCNE1G38S Polymorphism in Postoperative Atrial Fibrillation of North Indian Population: A Case-Control Study. (2017), *Biomed Pharmacol J.*, 10(3).
- Singh A, Singh P, Srivastava A.N., Akhtar S., Siddiqui M.H., Upadhyay S. Impact of MicroRNAs In Cancers–A Minireview (2017), *Int J of Biology, Pharmacy & Allied sciences*, 7(1).
- Ahmad S.S., Akhtar S., Rizvi S.M.D., Kamal M.A., Sayeed U., Khan M.K.A., Siddiqui M.H. & Arif J.M. Screening and Elucidation of Selected Natural Compounds for Anti-Alzheimer's Potential Targeting BACE-1 Enzyme: A Case Computational Study. (2017), *Curr Comput Aided Drug Des.*, 13(4):311-318 (Impact Factor = 1.639)
- Khan M.K.A., Akhtar S., Arif J.M., Structural Insight into the Mechanism of Dibenzo[a,l]pyrene and Benzo[a]pyrene-Mediated Cell Proliferation Using Molecular Docking Simulations.(2017), *Interdiscip Sci Comput Life Sci* 10(4):653-673 (Impact Factor = 3.492)
- Khan M.K.A., Akhtar S., Arif J.M., Development of In Silico Protocols to Predict Structural Insights into the Metabolic Activation Pathways of Xenobiotics. (2017), *Interdiscip Sci Comput Life Sci.* 10(2):329-345 (Impact Factor = 3.492)
- Shakeel E., Akhtar S., Khan M.K.A., Lohani M., Arif J.M., Siddiqui M.H. Molecular docking analysis of aplysin analogs targeting survivin protein. (2017), *Bioinformation*, 13 (9), 293-300 (PubMed Indexed).
- Sharma N., Akhtar S*, Jamal Q.M.S., Kamal M.A., Khan M.K.A, Siddiqui M.H., Sayeed U. Elucidation of antiangiogenic potential of Vitexin obtained from Cucumis sativus targeting Hsp90 protein: A

novel multipathway targeted approach to abstrain angiogenic phenomena (2017), *Medicinal Chemistry*, 13(3), 282-291. (Impact Factor = 2.329)

- Sayeed U., Wadhwa G., Jamal Q.M.S., Kamal, M.A., Akhtar S., Siddiqui, M.H. and Khan M.S. MHC binding peptides for designing of vaccines against Japanese encephalitis virus: A computational approach. (2018), *Saudi Journal of Biological Sciences*, 25(8), 1546-51. (Impact Factor = 4.052)
- Akhtar S., Khan M.K.A., Arif J.M., Evaluation and Elucidation Studies of Natural Aglycones for Anticancer Potential using Apoptosis-Related Markers: An Insilico Study (2018), *Interdiscip Sci Comput Life Sci* 10(2):297-310. (Impact Factor = 3.492)
- Yadav S., Akhtar S., Agarwal S.K., Majumdar G., Vimal S., Sharma M. IL-10(-592A/C) gene variant a predictor of postoperative atrial fibrillation in the north Indian population. (2018), *J Arrhythm.*, 34(3), 281-285.
- Sharma N., Sharma M., Shakeel E., Jamal Q.M.S., Kamal M.A., Khan M.K.A, Siddiqui M.H., Arif J.M., Sayeed U., Akhtar S*. Molecular Interaction and Computational Analytical Studies of Pinocembrin for its Antiangiogenic Potential Targeting VEGFR-2: A Persuader of Metastasis (2018), *Medicinal Chemistry*, 14, 1-15. (Impact Factor = 2.329)
- Sharma M., Pandey C., Sharma N., Kamal M.A., Sayeed U., Akhtar S.*. Cancer Nanotechnology - An Excursion on Drug Delivery Systems. (2018), *Anticancer Agents Med Chem.*, 18(15):2078-2092 (Impact Factor = 2.527)
- Shakeel E., Sharma N., Akhtar S., Khan M.K.A., Lohani M., Siddiqui M.H. Decoding the antineoplastic efficacy of Aplysin targeting Bcl-2: A *de novo* Perspective. (2018), *Computational Biology and Chemistry*, 77 (390-401) (Impact Factor = 3.737)
- Gupta C.L., Khan M.B., Ampasala D.R., Akhtar S., Dwivedi U.N., Bajpai P. Pharmacophore-based virtual screening approach for identification of potent natural modulatory compounds of human Toll-like receptor 7. (2019), *J Biomol Struct Dyn.*, Jan 21:1-16. (Impact Factor = 5.235)
- Saxena G., Akhtar S*, Sharma N., Sharma M., Siddiqui M.H. and Khan M KA. Virtual screening, docking and molecular dynamics simulation studies of selected phytochemical compounds against receptor tyrosine kinases: A correlative anti angiogenic study (2019), *Bioinformation*, 15(9): 613-620.
- Saxena G., Sharma N., Sharma M., Akhtar S*, Khan M KA and Siddiqui M.H. Global And Indian Scenario Of Cancer And Side Effects Induced By Various Anticancer Agents With An Overview To Recent Developments In Cure Of Cancer. (2019), *IJBPAS*, 8(9): 1749-1779.

- Saxena G., Sharma M., Sharma N., Khan MKA., Siddiqui M H and Akhtar S*. Molecular modeling and dynamics simulation studies of screened natural compounds: *1'-(4-(tert-butyl)benzoyl)spiro[chroman-2,4'-piperidin]-4-one and 3-(4-methylthiazol-2-yl)-2-oxo-2h-chromen-7-yl pivalate* targeting VEGFR-2 protein as potential anti-angiogenic agents. (2019), *J. Pharm. Sci. & Res.*, 11(7), 2495-2503.
- Maurya S., Akhtar S., Siddiqui M H and Khan M K A. Subtractive Proteomics for Identification of Drug Targets in Bacterial Pathogens: A Review (2020) *International Journal of Engineering Research & Technology*, 9 (01), 01-12
- Azim I., Akhtar S., Siddiqui M H., Khan M K A. Identification of Potential Lead Molecule against Sphingosine kinase-1: An in vitro study (2019). *Journal of Pharmaceutical Sciences and Research.*, 11 (12), 3790-3793
- Rehman A, Akhtar S, Siddiqui M H, Khan M K A. In Silico Identification of Drug-Like Inhibitors against Mtb-DHDDS: A Shape-Based Approach (2019) *Journal of Pharmaceutical Sciences and Research.*, 11 (5), 2084-2089.
- Shakeel E., Kumar R., Sharma N., Akhtar S., Khan A., Lohani M. and Siddiqui M H. Computational Outlook of Marine Compounds as Anti-Cancer Representatives Targeting BCL-2 and Survivin (2019) *Curr Comput Aided Drug Des.* 15 (3), 265-276. (Impact Factor = 1.639)
- Jamal, Q., Siddiqui, M.U., Alharbi, A.H., Albejaidi, F., Akhtar, S., Alzohairy, M.A., Kamal, M.A. and Kesari, K.K. A computational study of natural compounds from *Bacopa monnieri* in the treatment of Alzheimer's disease (2020). *Current Pharmaceutical Design*, 26(7), 790-800. (Impact Factor = 3.310)
- Sharma, N., Sharma, M., Sajid Jamal, Q.M., Kamal, M.A. and Akhtar, S*. Nanoinformatics and biomolecular nanomodeling: a novel move en route for effective cancer treatment (2020). *Environmental Science and Pollution Research*, 27(16), 19127-19141. (Impact Factor = 5.190)
- Umar, A.M., Akhtar S., Siddiqui M H. and Khan M K A. Identification of potential lead molecules against dibenzo [a, l] pyrene-induced mammary cancer through targeting cytochrome P450 1A1, 1A2, and 1B1 isozymes. (2021) *Biointerface Res Appl Chem*, 12(1), 1096-109.
- Rehman A., Akhtar S. and Khan M K A. Combinatorial design to decipher novel lead molecule against *Mycobacterium tuberculosis*. (2021) *Biointerface Res Appl Chem*, 11(5), 12993-3004.
- Khan M K A., Akhtar S., Al-Khodairy F., M Al-Marshad Feras, M A., Abdulrahman, Arif J M. Computational Exploration of dibenzo [a, l] pyrene Interaction to DNA and its Bases: possible Implications to Human Health. (2021) *Biointerface Res Appl Chem*, 11 11272-11283.

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- Khan I, Akhtar S. and Khan MKA. Lifestyle-based health awareness using digital gadgets and online interactive platforms. (2021) *NeuroPharmac J.*, 6(3): 295-310.
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- Awasthi K, Akhtar S., Khan MKA. Bioplastic: An accost towards sustainable development. (2021). *NeuroPharmac Journal.* 6, 162-168.
- Shah, A.A., Kamal, M.A. and Akhtar, S.* Tumor angiogenesis and VEGFR-2: mechanism, pathways and current biological therapeutic interventions. (2021). *Current Drug Metabolism*, 22(1), 50-59. (Impact Factor = 3.408)
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