Curriculum Vitae

Dr. Ajaykumar Gandhi
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Department of **Chemistry and Polymer Chemistry**,
Government College of Arts and Science
Near Subhedari Guest House, Kile Ark, Aurangabad
Maharashtra, India, 431004

Research Interests	Computer-Aided Drug Discovery, Ecotoxicology
ORCID:	https://orcid.org/0000-0002-2125-6596
Google Scholar Profile	https://scholar.google.com/citations?user=gGsa9S4AAAAJ&hl=en&authuser=1
Research Gate Profile	https://www.researchgate.net/profile/Ajaykumar-Gandhi

ACADEMIC RECORD

- PhD (Chemistry) : PhD Thesis Title: "Computer-Assisted Evaluation of Drug Candidates for Infectious Diseases, Cancer, and Metabolic Disorder: Proof of Concept Approach", Dr. Babasaheb Ambedkar Marathwada University, Aurangabad. August, 2022.
- UGC-CSIR-NET: June, 2010
- Post-Graduation: M.Sc. (Organic Chemistry), Savitribai Phule Pune University, Aurangabad. June, 2010

HONORS AND AWARDS

Nil

MEMBERSHIP:

- Life member of Indian Science Congress Association (ISCA)

REVIEWER/EDITOR

Nil

- **Research Experience**

❖ Research Projects And Grants Received As Investigator: Nil

❖ Publications:

1. **Ajaykumar Gandhi**, Vijay Masand, Magdi E. A. Zaki, Sami A. Al-Hussain, Anis Ben Ghorbal, Archana Chapolikar, *QSAR analysis of sodium glucose co–transporter 2 (SGLT2) inhibitors for anti-hyperglycaemic lead development*, SAR and QSAR in Environmental Research, 32:9, 731-744, DOI: 10.1080/1062936X.2021.1971295 Link to this article: https://doi.org/10.1080/1062936X.2021.1971295 (**Impact Factor: 3.000**)
2. **Ajaykumar Gandhi**, Vijay Masand, Magdi E. A. Zaki, Sami A. Al-Hussain, Anis Ben Ghorbal, Archana Chapolikar, *Quantitative Structure–Activity Relationship Evaluation of MDA-MB-231 Cell Anti-Proliferative Leads*, Molecules 2021, 26(16), 4795; DOI: 10.3390/molecules26164795. Link to this article: https://doi.org/10.3390/molecules26164795 (**Impact Factor: 4.411**)
3. Vijay H. Masand, Siddhartha Akasapu, **Ajaykumar Gandhi**, Vesna Rastija, Meghshyam K. Patil, Structure features of peptide-type SARS-CoV main protease inhibitors: Quantitative structure activity relationship study, Chemometrics and Intelligent Laboratory Systems, Volume 206, 2020, 104172, ISSN 0169-7439, DOI: 10.1016/j.chemolab.2020.104172 Link to this article: https://doi.org/10.1016/j.chemolab.2020.104172 (**Impact Factor: 3.491**)
4. V.H. Masand, V. Rastija, M.K. Patil, **Ajaykumar Gandhi** & Archana Chapolikar Extending the identification of structural features responsible for anti-SARS-CoV activity of peptide-type compounds using QSAR modelling, SAR and QSAR in Environmental Research, 31:9, 643-654, DOI: 10.1080/1062936X.2020.1784271 Link to the article: https://doi.org/10.1080/1062936X.2020.1784271 (**Impact Factor: 3.000**)
5. QSAR based virtual screening derived identification of a novel hit as a SARS CoV-229E $3CL^{pro}$ Inhibitor: GA-MLR QSAR modelling supported by molecular Docking, molecular dynamics simulation and MMGBSA calculation approaches (**Impact Factor: 3.000**)
6. Identification of Potent Aldose Reductase Inhibitors as Antidiabetic (Anti-hyperglycaemic) agents using QSAR Based Virtual Screening, Molecular Docking, MD Simulation and MMGBSA Approaches DOI: 10.1016/j.jsps.2022.04.003 (**Impact Factor: 3.000**)
7. QSAR, Molecular Docking, MD Simulation and MMGBSA Calculations Approaches to Recognize Concealed Pharmacophoric Features Requisite for the Optimization of ALK Tyrosine Kinase Inhibitors as Anticancer Leads https://doi.org/10.3390/molecules27154951 (**Impact Factor: 3.000**)
8. QSAR Evaluations to Unravel the Structural Features in Lysine-Specific Histone Demethylase 1A Inhibitors for Novel Anticancer Lead Development Supported by Molecular Docking, MD Simulation and MMGBSA https://doi.org/10.3390/molecules27154758 (**Impact Factor: 3.000**)

❖ Conference Papers

1. **Ajaykumar Gandhi**, Vijay Masand, Archana Chapolikar, International Conference On Multidisciplinary Aspects of Environment and Sustainable Development after Covid-19 Pandemic, *QSAR Evaluation of Amylase Inhibitors for the anti-Hyperglycemic Lead Development*
2. **Ajaykumar Gandhi**, Vijay Masand, Archana Chapolikar, *QSAR Evaluation of Glucagon Receptor (GCGR) Antagonists for the Anti-Hyperglycemic Lead Development*, Virtual International Conference on Multifunctional Advanced Materials organized by Department of Chemistry, Jnan Vikas Mandal's Degree College, Airoli and Association of Chemistry Teacher (ACT) C/o Homi Bhabha Centre for Science Education(TIFR) Mumbai, on 9-10th August 2021. (2nd Prize)
3. **Ajaykumar Gandhia**, Vijay Masand, Archana Chapolikara. Pharmacophore Modeling of some of the novel 1, 3, 4-thiadiazole derivatives, International Conference on Drug Discovery 2020, held at BITS-Hyderabad, 29th Feb - 2nd Mar 2020.

- **BOOKS:**

Edited Book Chapters

- **Recent Advances in Science and Economics, I***n Silico Evaluation of Bromodomain Family Protien Inhibitorsfor optimisation to thereauptic drug against Breast Cancer:A quantitative structure activity approach***, Pustak Bharti Toronto Canada M2R3E4, ISBN 978-1-989416-85-3.**
- **Recent Advances in Science and Technology,** *QSAR Evaluation of Amylase inhibitors for the antihyperglycemic lead development***, Pustak Bharti Toronto Canada M2R3E4, ISBN:978-1-989416-75-4.**

- **PATENTS**

Nil

- **PRESENTATIONS AND INVITED LECTURES**

❖ Paper (Poster/Oral) Presentation,

1. **Ajaykumar Gandhi**, Vijay Masand, Archana Chapolikar, International Conference On Multidisciplinary Aspects of Environment and Sustainable Development after Covid-19 Pandemic, *QSAR Evaluation of Amylase Inhibitors for the anti-Hyperglycemic Lead Development*
2. **Ajaykumar Gandhi**, Vijay Masand, Archana Chapolikar, *QSAR Evaluation of Glucagon Receptor (GCGR) Antagonists for the Anti-Hyperglycemic Lead Development*, Virtual International Conference on Multifunctional Advanced Materials organized by Department of Chemistry, Jnan Vikas Mandal's Degree College, Airoli and Association of Chemistry Teacher (ACT) C/o Homi Bhabha Centre for Science Education(TIFR) Mumbai, on 9-10th August 2021. (2nd Prize)
3. **Ajaykumar Gandhi**, Vijay Masand, Archana Chapolikara. *Pharmacophore Modeling of some of the novel 1, 3, 4-thiadiazole derivatives*, International Conference on Drug Discovery 2020, held at BITS-Hyderabad, 29th Feb - 2nd Mar 2020.

❖ Keynote Address,

- "Topic: *Applications of quantitative structure-toxicity relationship (QSTR) evaluation in ecotoxicological predictions,*" The second **International** Short Term Training Programme (ISTTP-2) will be conducted on Impact and Panacea of Environmental Pollution: The Past, Present and Future from 20th to 26th April 2022. (International within country)
- Emerging Trends and Practices in Environmental Conservation

❖ Workshop,

Nil

- **TEACHING EXPERIENCE**

PG: 00Years

UG: 05Years

- **PROFESSIONAL TRAINING**

- Foundation Training Programme for Class-I, Gazetted Officers of Higher and Technical Education Department, Yashwantrao Chavan Academy of Development Administration, Pune (YASHDA), 08/11/2017-19/12/2017, 42 Days
- STC, Developments in Advance drug Delivery Systems and Drug Discovery to Treat Life Threatening Diseases, Jawaharlal Nehru Technological University, Hyderabad, 22/06/2020 to 27/06/2020, 1 Week,
- STC, Challenges in Discovery of Antivirals and Vaccines, Jawaharlal Nehru Technological University, Hyderabad, 08/06/2020 to 13/06/2020,1 Week
- FDP, "ADVANCED CONCEPTS FOR DEVELOPING MOOCS" 02/07/2020 to 17/07/2020, Teaching Learning Centre, Ramanujan College, Delhi University, 2 Week
- Pre PhD Course work, Dr.Babasaheb Ambedkar Marathwada University, Aurangabad, 02/01/2021 To 15/02/2021, 45 days
- Maharashtra State Development of Educators and Enhancement in Delivery (MS-DEED) Program for Maharashtra State Science and Mathematics Teachers from Higher Education Institutes to be held by Centre of Excellence in Science and Mathematics Education (CoESME), at IISER Pune 25/04/2022-27/04/2022, Level-1, 03 Days

- 125th Orientation Programme, UGC-HRDC, Dr.Babasaheb Ambedkar Marathwada University, Aurangabad, 09-16/03/2020 & 15-26/06/2020, 21 days
- Online Refresher course in Chemistry for Higher Education, SAYAM ARPIT ONLINE COURSE, ("B" grade)

- **Professional Affiliations**

- **Professional Service**

- **Computer Skills**
  - MS-CIT
  - Softwares used: R , Marvin, Schrodinger, QSARINS, PyMOL, PyDescriptor, PaDEL, Molecular Docking softwares such as AutoDock, and molecular dynamic Simulation Softwares like Gromacs
  - Computer Languages: Python

- **Community ServicES**