

Allegato alla domanda di partecipazione
Curriculum formativo, didattico, scientifico e professionale del candidato

Dichiarazione sostitutiva di certificazioni

(Art. 46, D.P.R. 28 dicembre 2000 n. 445)

Dichiarazione sostitutiva dell'atto di notorietà

(da sottoscrivere davanti all'impiegato addetto o da presentare o spedire con la fotocopia di un documento di identità)
(Art. 47, D.P.R. 28 dicembre 2000 n. 445)

Estremi del bando di selezione	Codice Selezione n. 27A-21 AREA 02-Scienze Fisiche SC D1 SSD FIS07
Informazioni aggiornate al	02.07.2021
Nome e Cognome	Mohd Athar
Data di nascita	13th June 1991

Si raccomanda di indicare con precisione tutti gli elementi valutabili ai sensi del bando di selezione (aggiungere o togliere righe secondo necessità).

Esperienza professionale

Periodo	Ente	Principali attività e responsabilità
Feb-2019 to Dec-2020	Post-Doctoral Fellow	Maintaining small molecule databases, compilation of the high-throughput screening, optimization of the small molecule, virtual screening, predicting the targetability of the protein-target, Docking and SAR.
Dec-2020 to July-2021	Institute PostDoctoral Fellow	QM calculations of the fullerene-dyads, optoelectronics modeling, lipid-water interface interaction of the lipid monolayer.

Istruzione, formazione (es. titoli di studio, certificazioni professionali/linguistiche/informatiche)

Data	Titolo / Principali tematiche	Ente
22nd July 2011	B.Sc Biotechnology	
12 July 2013	M.Sc Applied Chemistry	
16th Oct 2019	Ph.D. Chemical Science (Computational chemistry)	
Oct 2016	Hands on Practice on LateX	
Feb 2016	Structure based Drug Design	
Sep 2012	Recent Advances In Computational Biology And Structural Based Drug Designing by Schrödinger	

Pubblicazioni / Convegni

- Kongor, A., Panchal, M., Athar, M., Vora, M., Makwana, B., Jha, P. C., & Jain, V. (2021). Calix [4] pyrrole stabilized PdNPs as an efficient heterogeneous catalyst for enhanced degradation of water-soluble carcinogenic Azo dyes. *Catalysis Letters*, 151(2), 548-558.
- Vora, M., Kongor, A., Panchal, M., Athar, M., Verma, A., Panjwani, & Jain, V. (2020). A highly selective anthraquinone appended oxacalixarene receptor for fluorescent ICT sensing of F⁻ ions: an experimental and computational study. *Journal of Chemical Sciences*, 132(1), 1-10.
- Patel, D., Athar, M., & Jha, P. C. (2020). Computational investigation of binding of chloroquinone and

- hydroxychloroquinone against PLPro of SARS-CoV-2. *Journal of Biomolecular Structure and Dynamics*, 1-11.
4. Kongor, A., Panchal, M., Athar, M., Vora, M., Verma, N., Pandya, A., & Jain, V. (2020). Colorimetric and electrochemical sensing of As (III) using calix [4] pyrrole capped gold nanoparticles and evaluation of its cytotoxic activity. *Journal of Inclusion Phenomena and Macrocyclic Chemistry*, 98(1), 29-41.
 5. Panchal, M., Kongor, A., Athar, M., Modi, K., Patel, C., Dey, S., & Jain, V. K. (2020). Structural motifs of oxacalix [4] arene for molecular recognition of nitroaromatic explosives: Experimental and computational investigations of host-guest complexes. *Journal of Molecular Liquids*, 112809.
 6. Kongor, A., Panchal, M., Athar, M., Bhatt, K., Jha, P. C., & Jain, V. (2019). Facile construction of calix [4] pyrrole-templated gold nanoparticles: computational insights and application for efficient reduction of 4-nitrophenol. *Gold Bulletin*, 52(3-4), 125-133.
 7. Sharma, V. S., Sharma, A. S., Shah, A. P., Shah, P. A., Shrivastav, P. S., & Athar, M. (2019). New Class of Supramolecular Bowl-Shaped Columnar Mesogens Derived from Thiocalix [4] arene Exhibiting Gelation and Organic Light-Emitting Diodes Applications. *ACS omega*, 4(14), 15862-15872.
 8. Athar, M., & Jha, P. C. (2019) DFT study of guest-responsive cooperative effects: Inclusion complexation of alcohols with calix[4]pyrrole, *Monatshefte für Chemie - Chemical Monthly*. 150, (7) 1205–1214
 9. Sinha, S., Patel, S., Athar, M., Vora, J., Chhabria, M.T., Jha, P.C. and Shrivastava, N., (2019). Structure-based identification of novel sirtuin inhibitors against triple negative breast cancer: An in silico and in vitro study. *International journal of biological macromolecules*. 140, 454-568.
 10. Athar, M., Das Soubhik, Jha PC et al., (2018). Conformational Equilibrium Study of Calix[4]tetrolarenes using Density Functional Theory (DFT) and Molecular Dynamics Simulations, *Supramolecular Chemistry*. 30, 12, 982-993
 11. Shah, D. J., Sharma, A. S., Shah, A. P., Sharma, V. S., Athar, M., & Soni, J. Y. (2019). Fixation of CO₂ as a carboxylic acid precursor by microcrystalline cellulose (MCC) supported Ag NPs: a more efficient, sustainable, biodegradable and eco-friendly catalyst. *New Journal of Chemistry*, 43(22), 8669-8676.
 12. Vora, J., Patel, S., Athar, M., Sinha, S., Chhabria, M. T., Jha, P. C., & Shrivastava, N. (2019). Pharmacophore modeling, molecular docking and molecular dynamics simulation for screening and identifying anti-dengue phytocompounds. *Journal of Biomolecular Structure and Dynamics*, 1-15.
 13. Athar, M., Das Soubhik, Jha PC et al., (2018). Conformational Equilibrium Study of Calix[4]tetrolarenes using Density Functional Theory (DFT) and Molecular Dynamics Simulations, *Supramolecular Chemistry*. 30, 12, 982-993 <https://doi.org/10.1080/10610278.2018.1517876>
 14. Athar, M., Ranjan, P., & Jha, P. C. (2018). A DFT study of inclusion complexes of substituted calix [n] arenes with dasatinib and lapatinib. *Journal of molecular graphics & modelling*, 84, 160-165. <https://doi.org/10.1016/j.jmgm.2018.06.018>
 15. Kongor, A., Panchal, M., Athar, M., Jha, P. C., Jhala, D., Sindhav, G., & Jain, V. (2018). Selective fluorescence sensing of Cu (II) ions using calix [4] pyrrole fabricated Ag nanoparticles: A spectroscopic and computational approach. *Journal of Molecular Liquids*. 269, 467-475. <https://doi.org/10.1016/j.molliq.2018.08.014>
 16. Ranjan, P., Athar, M., Rather, H., Vijayakrishna, K., Vasita, R., & Jha, P. C. (2018). Rational design of imidazolium based salts as anthelmintic agents: A combination of experimental and in-silico approach. 255, 578-588 *Journal of Molecular Liquids*. <https://doi.org/10.1016/j.molliq.2018.02.001>
 17. Bhatt Keyur., Kongor, A., Athar M., (2018). Functionalized Calixarenes Drug-Sensing Receptor: A Review, *Medicinal & Analytical Chemistry International Journal*, 2 (2), 1-4.
 18. Kongor, A., Panchal, M., Athar, M., Mehta, V., Bhatt, K., Jha, P. C., & Jain, (2018) Synthesis and modeling of calix[4]pyrrole wrapped Au nanoprobe for specific detection of Pb(II): Antioxidant and radical scavenging efficiencies, *Journal of Photochemistry and Photobiology A: Chemistry*. 364, 801-810. <https://doi.org/10.1016/j.jphotochem.2018.07.024>
 19. Ranjan, P., Athar, M., Vijayakrishna, K., Meena, L. K., Vasita, R., & Jha, P. C. (2018). Deciphering the anthelmintic activity of benzimidazolium salts by experimental and in-silico studies. *Journal of Molecular Liquids*. 256, 156-168. <https://doi.org/10.1016/j.molliq.2018.07.029>
 20. Ranjan, P., Athar, M., Vijayakrishna, K., & Jha, P. C. (2018). Probing the opportunities for designing Anthelmintic leads by Sub-Structural Topology Based QSAR Modelling. *Molecular Diversity* 22 (3), 669-683. <https://doi.org/10.1007/s11030-018-9825-4>

21. Patel K Saumya, Athar, M. et al., (2018) Assessing the Antimalarial Potentials of Phytochemicals: Virtual Screening, Molecular Dynamics and In-Vitro Investigations *Letters in Drug Design & Discovery* 0.2174/1570180815666180604085626 (Equal Authorship)
22. Kongor, A., Panchal, M., Athar, M., Mehta, V., Bhatt, K., Jha, P. C., & Jain, V. (2017). Heterogeneous hydrogenation using stable and reusable calix [4] pyrrole fenced Pt nanoparticles and its mechanistic insight. 437, 195-201. *Applied Surface Science*. <https://doi.org/10.1016/j.apsusc.2017.12.172>
23. Athar, M., Lone, M. Y., & Jha, P. C. (2017). Recognition of Anions using urea and thiourea substituted calixarenes: A DFT assessment of Non-Covalent Interactions. *Chemical Physics* 501, 68-77. <https://doi.org/10.1016/j.chemphys.2017.12.002>
24. Athar, M., Lone, M. Y., & Jha, P. C. (2018). Designing of Calixarene based Drug Carrier for Dasatinib, Lapatinib and Nilotinib using Multilevel Molecular Docking, Semiempirical and Dynamics Simulations, *Journal of Inclusion Phenomena and Macrocyclic Chemistry*. 90, 157-169 <https://doi.org/10.1007/s10847-017-0773-x>
25. Mohsin Y Lone, S Prashant Kumar, Mohd Athar, Prakash C Jha. (2017) Exploration of Mycobacterium tuberculosis Structural Proteome: An In-silico Approach. *Journal of Theoretical Biology* 439, 14-23. <https://doi.org/10.1016/j.jtbi.2017.11.021>
26. Athar M, Kongor A, Panchal M, Jha PC, Jain V (2017) Entrapment of Toxic Anions Using Calixarenes framework. *MOJ Toxicol* 3(6): 00074. <http://dx.doi.org/10.15406/mojt.2017.03.00074>
27. Panchal, M. K.; Kongor, A.; Athar, M.; Mehta, V. A.; Jha, P. C.; Jain, V. K., (2017). Sensing of Ce(III) using dinaphthoylated oxacalix[4]arene via realistic simulations and experimental studies. *New Journal of Chemistry*. 42, 311-317 <http://dx.doi.org/10.1039/C7NJ02828H>
28. Lone, M. Y., Manhas, A., Athar, M., & Jha, P. C. (2017). In Silico Exploration of Vinca Domain Tubulin Inhibitors: A Combination of 3D-QSAR-Based Pharmacophore Modeling, Docking and Molecular Dynamics Simulations, *ChemistrySelect* 2(33) 10848 <http://dx.doi.org/10.1002/slct.201701971>
29. Athar, M., Lone, M. Y., & Jha, P. C. (2017). Investigation of structure and conformational equilibrium of Oxacalix [4] arene: A density functional theory approach. *Journal of Molecular Liquids*. 237, 473-483. <http://dx.doi.org/10.1016/j.molliq.2017.04.065>
30. Athar, M., Lone, M. Y., & Jha, P. C. (2017). First protein drug target's appraisal of lead-likeness descriptors to unfold the intervening chemical space. *Journal of Molecular Graphics and Modelling* 72, 272-282. <http://dx.doi.org/10.1016/j.jmgm.2016.12.019>
31. Athar M., Lone, M. Y., Khedkar, V. M., & Jha, P. C et al, (2017). Structural Investigation of Vinca domain tubulin binders by Pharmacophore, Atom based QSAR, Docking and Molecular Dynamics Simulations, *Combinatorial Chemistry & High Throughput Screening*, volume 20. 8, 682-695. <http://dx.doi.org/10.2174/1386207320666170509151253>
32. Lone, M. Y., Athar, M., & Jha, P. C. Gupta VK, (2017). Prioritization of natural compounds against mycobacterium tuberculosis 3-dehydroquinase dehydratase: A combined in-silico and in-vitro study, *Biochemical and Biophysical Research Communications*, 491 (4) 1105-1111. <https://doi.org/10.1016/j.bbrc.2017.08.020>.
33. Athar, M., Lone, M. Y., & Jha, P. C. (2017). Theoretical assessment of calix[n]arene as drug carriers for second generation tyrosine kinase inhibitors, *Journal of Molecular Liquids*, 247, 448-455. <http://dx.doi.org/10.1016/j.molliq.2017.09.113>
34. Lone, M. Y., Athar, M., & Jha, P. C. Gupta VK, (2017). Identification of Mycobacterium tuberculosis enoyl-acyl carrier protein reductase inhibitors: A combined in-silico and in-vitro analysis. *Journal of Molecular Graphics and Modelling* 76 172-180. <http://dx.doi.org/10.1016/j.jmgm.2017.07.005>.
35. Lone, M. Y., Manhas, A., Athar, M., & Jha, P. C. (2017). Identification of InhA Inhibitors: A Combination of Virtual Screening, Molecular Dynamics Simulations and Quantum Chemical Studies. *Journal of Biomolecular Structure and Dynamics*, (just-accepted), 1-59. <http://dx.doi.org/10.1080/07391102.2017.1372313>
36. Panchal, M., Athar, M., Jha, P. C., Kongor, A., Mehta, V., Bhatt, K., & Jain, V. K , (2017), Quinoline appended oxacalixarene as turn-off fluorescent probe for the selective and sensitive determination of Cu ions: A combined experimental and DFT study, *Journal of Luminescence*, Volume 192, Pages 256-262, ISSN 0022-2313, <http://dx.doi.org/10.1016/j.jlumin.2017.06.052>

37. Mehta, V., Athar, M., Jha, P. C., Panchal, M., Modi, K., & Jain, V. K. (2017). Turn-Off^o Fluorescence sensor for insensitive munition using anthraquinone appended oxacalix[4]arene and its computational studies, *New Journal of Chemistry*, 41, 5125-5132 <http://dx.doi.org/10.1039/C7NJ01111>
38. Panchal, M., Athar, M., Jha, P. C., Kongor, A., Mehta, V., Bhatt, K., & Jain, V. K. (2016). Turn-off fluorescence probe for the selective determination of pendimethalin using a mechanistic docking model of novel oxacalix [4] arene. *RSC Advances*, 6(58), 53573-53577. <http://dx.doi.org/10.1039/C6RA05707A>
39. Mehta, V., Athar, M., Jha, P. C., Panchal, M., Modi, K., & Jain, V. K. (2016). Efficiently functionalized oxacalix [4] arenes: Synthesis, characterization and exploration of their biological profile as novel HDAC inhibitors. *Bioorganic & medicinal chemistry letters*, 26(3), 1005-1010. <http://dx.doi.org/10.1016/j.bmcl.2015.12.044>
40. Athar, M., Lone, M. Y., Khedkar, V. M., & Jha, P. C. (2016). Pharmacophore model prediction, 3D-QSAR and molecular docking studies on vinyl sulfones targeting Nrf2-mediated gene transcription intended for anti-Parkinson drug design. *Journal of Biomolecular Structure and Dynamics*, 34(6), 1282-1297. <http://dx.doi.org/10.1080/07391102.2015.1077343>
41. Mohd Athar, Amar Jyoti Das (2014). Therapeutic nanoparticles: State-of-the-art of nanomedicine. *Advanced Material Reviews*, 1 (1). <http://dx.doi.org/10.5185/amr.2014.1005>
42. Athar M, Sona AM, Bekono BD, Fidele NK; (2019), Fundamental physical and chemical concepts behind "drug-likeness" and "natural product-likeness". *Cheminformatics of Natural Products, Physical Sciences Reviews*. 20180101. DeGruyter.
43. Koulouridi E, Athar M. et al, (2019) Glossary of terms used in chemoinformatics of natural products: fundamental principles, *Cheminformatics of Natural Products, Physical Sciences Reviews*. DeGruyter.
44. Kongor K, Panchal M, Athar M, Jain VK, (2019) Calix- Assisted Fabrication of Metal Nanoparticle s: Applications and Theoretical Insights, *21st Century Nanoscience – A Handbook (Volume 2)*. Taylor Francis 15-1, 15-14.

Altre attività scientifiche

Actively involved in reviewing activities of journals such as *Journal of Biomolecular structure and dynamics*, *Physical Science Reviews*, *Computational Biology and Chemistry* and *Journal of Molecular structure*.

Ulteriori informazioni pertinenti

--No-

Luogo, data e firma