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	CALL FOR NR. 1 RESEARCH GRANT ART. 22 L. 240/2010 02 - PHYSICS - SSD FIS/07 CALL SECT. 02/D1 APPLIED PHYSICS, PHYSICS TEACHING AND HISTORY OF PHYSICS
Informazioni aggiornate al	01.09.2022
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**
Aug-2021 to July2022	Post-Doctoral Fellow	All atom/Coarse Grain Molecular Dynamics simulations and Docking for the project entitled "Studio computazionale dell'interazione di inibitori con sistemi di efflusso batterici"
4-02-2019 to 13- 12-2020	Post-Doctoral Fellow	Maintaing small molecule databases, compilation of the high-thoroughput screening, optimization of the small molecule, virtual screening, predicting the targetability of the protein-target, Docking and SAR.
14-12-2020 to 05-08-2021	Institute PostDoctoral Fellow	QM calculations of the fullerene-dyads, optoelectronics modeling, lipid-water interface interation 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

1. **Athar, M.,** & Patnaik A. (2022). Through-Bond Driven Through-Space Interactions in a Fullerene C60 Non-Covalent Dyad: Unusual Strong Binding between Spherical and Planar π Electron Clouds

and Culmination of Dyadic Fractals. The Journal of Physical Chemistry A. 126, 23, 3629–3641

2. Patel, D.#, **Athar, M**.#, & Jha, P. C. (2021). Exploring Ruthenium-based organometallic inhibitors against Plasmodium Calcium Dependent Kinase 2 (PfCDPK2): a combined ensemble docking, QM/MM and molecular dynamics study. ChemistrySelect. 6, 32, 8189-8199. (*Equal Contribution)*

3. 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.

4. 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.

5. 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.

6. 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.

7. 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.

8. 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.

9. 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 Thiacalix [4] arene Exhibiting Gelation and Organic Light-Emitting Diodes Applications. *ACS omega*, *4*(14), 15862-15872.

10. **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

11. 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.

12. **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

13. 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.

14. 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.

15. **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

16. **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

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. 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)

19. 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

20. **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

21. **Athar**, M., Lone, M. Y., & Jha, P. C. (2018). Designing of Calixarene based Drug Carrier for Dasatinib, Lapatinib and Nilotinib using Multilevel Molecular Docking, Semiemperical and Dynamics Simulations, *Journal of Inclusion Phenomena and Macrocyclic Chemistry.* 90, 157-169 https://doi.org/10.1007/s10847-017-0773-x

22. 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

23. **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

24. Panchal, M. K.; Kongor, A.; **Athar**, M.; Mehta, V. A.; Jha, P. C.; Jain, V. K., (2017). Sensing of Ce(III) using di-naphthoylated oxacalix[4]arene via realistic simulations and experimental studies. *New Journal of Chemistry*. **42**, 311-317 http://dx.doi.org/10.1039/C7NJ02828H

25. 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

26. **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

27. **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

28. **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

29. Lone, M. Y., **Athar**, M., & Jha, P. C. Gupta VK, (2017). Prioritization of natural compounds against mycobacterium tuberculosis 3-dehydroquinate 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.

30. **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

31. 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.

32. 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

33. **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

34. 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

35. 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.

36. 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

I am 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