

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	DIP. PHYSICS - Call for research grant N. 7/2022
Informazioni aggiornate al	23.06.2022
Nome e Cognome	Mohd Athar
Data di nascita	

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	InStem, NCBS Campus, India	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	Indian Institute of Technology Madras, India	Institute PostDoctoral Fellow: QM calculations of the fullerene-dyads, optoelectronics modeling, lipid-water interface interaction of the lipid monolayer.
Aug 2021 to July 2022	University of Cagliari, Italy	Post-Doctoral Fellow: Atomistic and coarse-grained simulations for understanding molecular details on the inhibition of the major efflux transporters in Gram-negative bacteria

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

Data	Titolo / Principali tematiche	Ente
22nd July 2011	B.Sc Biotechnology	Hemwati Nandan Bahuguna Garhwal University, India
12 July 2013	M.Sc Applied Chemistry	BabaSaheb Bhimrao Ambedkar University, India
16th Oct 2019	Ph.D. Chemical Science (Computational chemistry)	Central University of Gujarat, India
Oct 2016	Hands on Practice on LaTeX	SVNIT, India
Feb 2016	Structure based Drug Design	Schrodinger Inc.
Sep 2012	Recent Advances In Computational Biology And Structural Based Drug Designing by Schrödinger	Indian Institute of Information Technology, India

Pubblicazioni / Convegni

- Athar, M., & Patnaik, A. (2022). Through-Bond-Driven Through-Space Interactions in a Fullerene C60 Noncovalent Dyad: An 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.
- Patel, D., Athar, M., & Jha, P. C. (2022). Computational investigation of binding of chloroquinone and hydroxychloroquinone against PLPro of SARS-CoV-2. *Journal of Biomolecular Structure and Dynamics*, 40(7), 3071-3081 [Equal contribution].
- Patel, D., Athar, M., & Jha, P. C. (2021). Exploring Ruthenium-Based Organometallic Inhibitors against Plasmodium falciparum Calcium Dependent Kinase 2 (PfCDPK2): A Combined Ensemble Docking,

QM/MM and Molecular Dynamics Study. *ChemistrySelect*, 6(32), 8189-8199 [Equal contribution].

4. 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.
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. Shama, 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.
7. **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
8. 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.
9. **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
10. Shah, D. J., Shama, A. S., Shah, A. P., Shama, 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.

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