

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	22.03.2024
Nome e Cognome	Ruqaiya Khalil
Data di nascita	15th June 1990

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
Nov 2023 – to date	Senior Researcher, University of Karachi Computational Chemistry Lab	Development of novel insulin secretagogues from natural products
Mar 2023 – Jul 2023	Senior Researcher, Fundació Bosch i Gimpera, University of Barcelona	Benchmarking and automation protocols for Virtual screening. Management of molecular modeling projects for industrial partner
Sep 2021 – Jan 2023	Postdoctoral Fellow University of Vigo Centro De Investigaciones Biomédicas (CINBIO)	Analysis of the extensive all-atom MD simulations to analyze protein-ligand interactions, and mutation effects in protease-substrate complexes
Nov 2020 – Aug 2021	Postdoctoral Fellow, University of Karachi Center for Artificial Intelligence in Healthcare	Application of graph-based theory for classification, virtual screening, and lead optimization of the in-house compound database
Sep 2017 – Mar 201	Visiting Scholar, University of Copenhagen Department of Drug Design and Pharmacology	Homology modeling, docking, and all-atom molecular dynamics simulations to understand substrate binding in proton coupled oligopeptide receptors

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

Data	Titolo / Principali tematiche	Ente
Jan 2009 – Dec 2011	B.Sc Biochemistry	University of Karachi
Jan 2012 – Mar 2013	M.Sc Biochemistry	University of Karachi
Aug 2013 – Nov 2019	Ph.D. Molecular Medicine (Computational chemistry)	University of Karachi

Pubblicazioni / Convegni

1. Sajid S, Nielsen MMK, Khalil R , Hansen PR, Franzyk H, Jørgensen MG, Christensen LP, et al. 2023. Substrate space analysis of the bacterial proton-coupled oligopeptide transporter YdgR by cheminformatics. <i>FEMS Microbiol Lett.</i> , fnad052.

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66047776. **Ferreiro D, Khalil R, Gallego MJ, Osorio NS, and Arenas M.** 2022. The evolution of the HIV-1 protease folding stability. *Virus Evol.*, 8(2), veac115.
66049616. **Ali N, Khalil R, Nur-e-Alam M, Ahmed S, and Ul-Haq Z.** 2022. Probing the Mechanism of Peptide Binding to REV Response Element RNA of HIV-1; MD Simulations and Free Energy Calculations. *J Biomol Struct Dyn.*, 40(10), 4399–4408.
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66046176. **Khalil R, Usmani S, Nur-e-Alam M, Ahmed S, and Ul-Haq Z.** 2021. Site-directed Fragnomics and MD Simulations Approaches to Identify Interleukin-2 Inhibitors. *Med Chem.*, 17(4), 407–417.
66046336. **Gul S, Khalil R, Ul-Haq Z, and Mubarak MS.** 2020. Computational overview of mycobacterial thymidine monophosphate kinase. *Curr Pharm Des.*, 26(15), 1676–1681.
66048256. **Aduri NG, Montefiori M, Khalil R, Gajhede M, Jørgensen FS, and Mirza O.** 2019. Molecular Dynamics Simulations Reveal the Proton: Peptide Coupling Mechanism in the Bacterial Proton-Coupled Oligopeptide Transporter YBGH. *ACS Omega*, 4(1), 2040–2046.
66045856. **Khalil R, Ashraf S, Khalid A, and Ul-Haq Z.** 2019. Exploring novel N-myristoyltransferase inhibitors: A molecular dynamics simulation approach. *ACS omega*, 4(9), 13658–13670.
66045376. **Naz S, Baig N, Khalil R, and Ul-Haq Z.** 2019. Characterization of cryptic allosteric site at IL-4R α : new paradigm towards IL-4/IL-4R inhibition. *Int J Biol Macromol.*, 123, 239–245.
66046256. **Hammad A, Khan MA, Ahmad I, Imran A, Khalil R, Al-Adhami T, Rahman KM, et al.** 2020. Probing sulphamethazine and sulphamethoxazole based Schiff bases as urease inhibitors; synthesis, characterization, molecular docking and ADME evaluation. *Bioorg Chem.*, 105, 104336.
66047616. **Bano B, Khan KM, Begum F, Lodhi MA, Salar U, Khalil R, Ul-Haq Z, et al.** 2018. Benzylidene Indane-1, 3-Diones: as Novel Urease Inhibitors; Synthesis, In Vitro, and In Silico Studies. *Bioorg Chem.*, 81, 658–671
66048416. **Barakat A, Ali M, Al-Majid AM, Yousuf S, Choudhary MI, Khalil R, and Ul-Haq, Z.** 2017. Synthesis of thiobarbituric acid derivatives: in vitro α -glucosidase inhibition and molecular docking studies. *Bioorg Chem.*, 75, 99–105. Academic Press.
66048576. **Farooq M, Usman F, Naseem M, Aati HY, Ahmad H, Manee S, Khalil R, et al.** 2023. Voriconazole Cyclodextrin Based Polymeric Nanobeads for Enhanced Solubility and Activity: In Vitro/In Vivo and Molecular Simulation Approach. *Pharmaceutics*, 15(2), 389.
66048736. **Shah MA, Khalil R, Ul-Haq Z, and Panichayupakaranant P.** 2017. α -Glucosidase inhibitory effect of rhinacanthins-rich extract from Rhinacanthus nasutus leaf and synergistic effect in combination with acarbose. *J. Funct. Foods.*, 36, 325–331.
66048816. **Hamad A, Khan MA, Ahmad I, Khalil R, Khalid M, Abbas U, Azhar R, et al.** 2021. Bio-oriented synthesis of new sulphadiazine derivatives for urease inhibition and their pharmacokinetic analysis. *Sci Rep.*, 11(1), 18973.
66049216. **Shah S, Javaid K, Zafar H, Khan KM, Khalil R, Ul-Haq Z, Perveen S, et al.** 2018. Synthesis, and In vitro and in silico α -glucosidase inhibitory studies of 5-chloro-2-aryl benzo [d] thiazoles. *Bioorg. Chem.*, 78, 269–279.

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66045456. Sherwani ZA, **Khalil R**, Nur-e-Alam M, Ahmed S, Ul-Haq Z. 2022. Structure-based virtual screening to identify negative allosteric modulators of NMDA. *Med chem.*, 18(9), 990–1000.
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66045616. Madhumanchi S, Suedee R, Kaewpiboon S, Srichana T, **Khalil R**, Ul-Haq Z. 2020. Effect of sodium deoxycholate sulfate on outer membrane permeability and neutralization of bacterial lipopolysaccharides by polymyxin B formulations. *Int J Pharm.*, 581, 119265.
66045696. Seraj F, Kanwal, Khan KM, Khan A, Ali M, **Khalil R**, Ul-Haq Z, et al. 2021. Biology-oriented drug synthesis (BIODS), in vitro urease inhibitory activity, and in silico studies on ibuprofen derivatives. *Mol Diver.*, 25, 143–157.
66051776. Shah HS, Usman F, Ashfaq-Khan M, **Khalil R**, Ul-Haq Z, Mushtaq A, Qaiser R, et al. 2020. Preparation and characterization of anticancer niosomal withaferin--A formulation for improved delivery to cancer cells: In vitro, in vivo, and in silico evaluation. *J. Drug Deliv. Sci. Technol.*, 59, 101863.
66050656. Shah MA, Muhammad H, Mehmood Y, **Khalil R**, Ul-Haq Z, and Panichayupakaranant P. 2017. Superoxide scavenging and antiglycation activity of rhinacanthins-rich extract obtained from the leaves of *Rhinacanthus nasutus*. *Pharmacogn. Mag.*, 13(52), 652.
66051696. Shah MA, Reanmongkol W, Radenahmad N, **Khalil R**, Ul-Haq Z, and Panichayupakaranant P. 2019. Anti-hyperglycemic and anti-hyperlipidemic effects of rhinacanthins-rich extract from *Rhinacanthus nasutus* leaves in nicotinamide-streptozotocin induced diabetic rats. *Biomed. Pharmacother.*, 113, 108702.
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Altre attività scientifiche

I am actively involved in reviewing activities of journals including *Molecular Diversity*, *Journal of Molecular structure* and *Natural Product journal*.

Ulteriori informazioni pertinenti

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Luogo, data e firma