



# Mohammed Fouad

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## ABOUT ME

Graduate researcher with applied knowledge in **QSAR**, **cheminformatics**, and **molecular modelling** for drug discovery. Skilled in **machine learning** with Python, **RDKit** workflows, and experimental **antimicrobial evaluation**. Aiming to develop computational tools to accelerate drug design.

## EDUCATION AND TRAINING

1 SEP 2020 – 30 SEP 2024 Cairo, Egypt

**B.SC. IN CHEMISTRY** Al-Azhar University

**Key coursework:** Quantum & Physical Chemistry, Organic Chemistry, Inorganic Chemistry, Spectroscopy, Linear Algebra, Calculus, Statistics, Programming (Python), Physics.

**Thesis highlights:** Addressed a critical environmental issue by mitigating harmful gas emissions (nitrous oxide, carbon monoxide) from rice straw burning in Egypt through a three-step protocol (cellulose extraction, chemical activation, electrode fabrication).

**Thesis Grade:** (Very Good)

**Final grade** 67.64% | **Thesis** Cellulose-Based Electrode for Supercapacitors: Harnessing Rice Straw for Sustainable Energy Storage

## PUBLICATIONS

2026

**[Amphiphilic cellulose and alginate-functionalized magnetic ZIF-8 nanocomposites for dinitrophenol removal, colorimetric H<sub>2</sub>O<sub>2</sub> sensing, and antibacterial applications](#)**

### Highlights:

- Fe<sub>3</sub>O<sub>4</sub>/CRQ/ZIF-8 achieved 98.7% removal of 2,4-DNP with an adsorption capacity of 103.5 mg g<sup>-1</sup>.
- Fe<sub>3</sub>O<sub>4</sub>/CRQ/ZIF-8 nanozyme exhibited lower K<sub>m</sub> values than natural HRP.
- A portable hydrogel kit enabled visual H<sub>2</sub>O<sub>2</sub> detection with LOD ≈ 0.88 μM.
- Fe<sub>3</sub>O<sub>4</sub>/CRQ/ZIF-8 hydrogel coatings achieved 98.53% antibacterial inhibition.

**Authors:** Salah M. Tawfik; Hyejin Jang; Hyukjoo Kwon; Mohamed Fekry; Asmaa A. Roshdy; Ahmed Ragab; Belal Zakaria; Mohammed Fouad; Yousry A. Ammar; Moustafa S. Abusaif; Hoon Eui Jeong | **Journal Name:** International Journal of Biological Macromolecules

2026

**Quinoline and Quinolone Derivatives as Antimicrobial Agents: A Comparative Review of Synthesis, Reactivity, and SAR Insights.**

**Authors:** Mohammed Fouad; Zeinab A. Ibrahim; Mahmoud A. Diab; Mohamed El-Gnainy; Ahmed Ragab | **Journal Name:** Manuscript in Preparation

2026

**Design and Predict the Potential of Pyrazole-based Anti-Inflammatory agents using Fingerprint Machine Learning**

**Authors:** Mohamed M. Elsenety; Mohammed Fouad; Ahmed Ragab | **Journal Name:** In Progress

2026

**Eco-Friendly Synthesis of Chitosan-Silver Nanoparticles-Based Drug Delivery System for Cancer Treatment**

**Authors:** Nada Hisham; Zeinab A. Ibrahim; Fatma Ahmed; Mohammed Fouad; Mohamed Shaban | **Journal Name:** In Progress

## PROJECTS

### Ligand-Based Drug Design | 9th ADD Workshop Challenge, Palacký University Olomouc, Czech Republic

Our team built an RDKit-based pipeline to screen a 3,500-compound library: Morgan fingerprints, Tanimoto triage, Butina clustering, Lipinski/ADMET filtering, and docking-based rank-sum consensus. The final selection used a custom consensus plot to prioritize the top 100 leads.

Link <https://github.com/Mohaammed-Fouad/Ligand-Based-Virtual-Screening>

### Activity Prediction Against Aromatase Enzyme (ChEMBL 1978)

Developed and validated fingerprint-based ML models to predict anticancer activity using ChEMBL data. Included feature selection, cross-validation, and SHAP-based interpretability.

Link [https://github.com/Mohaammed-Fouad/Activity\\_prediction\\_against\\_aromatase\\_ChEMBL1978](https://github.com/Mohaammed-Fouad/Activity_prediction_against_aromatase_ChEMBL1978)

## INTERSHIPS

26 JAN 2026 – 30 JAN 2026

### 9th In-Silico Drug Design Workshop, Palacký University Olomouc | Online

Training in structure-based and ligand-based drug design (docking, MD, pharmacophores, QSAR, de novo design, ML), culminating in a ligand-selection challenge for compounds whose hits were ordered.

26 JAN 2026 – 30 JAN 2026

### Virtual Winter School on Computational Chemistry, CECAM | Online

Participated in an international virtual school offering a series of live lectures on foundational and advanced computational chemistry topics, including quantum chemistry, molecular dynamics, practical GROMACS and Q-Chem workshops, and research presentations.

30 AUG 2025 – 5 SEP 2025

### Drug Research Center, The British University in Egypt (BUE) | El-Sherouk, Egypt

Contributed to CADD-driven projects by running molecular docking (MzDock) and assisting experimental assays (cell culture, PCR, HPLC).

1 SEP 2023 – 15 SEP 2023

### Egyptian Atomic Energy Authority | Sharkia, Egypt

Applied UV-Vis, titrimetry, and HPLC for water treatment analysis; improved sample prep and data interpretation skills.

1 JUN 2023 – 1 NOV 2023

### McKinsey Forward Program | McKinsey & Company | New York, USA

Completed the 10-week Forward Core track and progressed to the 12-week Advanced level with virtual leadership workshops (e.g., Think Forward), team case work, and coach feedback.

## WORK EXPERIENCE

### STEM AND ROBOTICS COACH – I SHINE ACADEMY TECHNO KIDS TECHNO FUTURE – 20 Oct 2024 – 10 Jun 2025 – SHARKIA, EGYPT

Mentored **30+ students** in **reading research papers** and developing project ideas, and led a team that won **3<sup>rd</sup> place** in the First Lego League Challenge Competition.

## COURSES

1 AUG 2025 – 4 AUG 2025

### Python for Cheminformatics-Driven Molecular Docking | RCSB PDB, MolSSI

29 MAR 2025 – 29 MAY 2025

### Introduction to Data Science with Python | HarvardX, edX

7 JUN 2024 – 7 JUL 2024  
Ask Questions to Make Data-Driven Decisions | Google, Coursera

25 MAY 2024 – 6 JUN 2024  
Foundations: Data, Data, Everywhere | Google, Coursera

20 MAY 2024 – 20 JUN 2024  
CS50’s Introduction to Programming with Python | HarvardX, edX

1 SEP 2023 – 5 SEP 2023  
AI in drug discovery | I-mole Lab, Online

**VOLUNTEERING**

1 JAN 2025 – CURRENT Remote  
CEO - URS Scholarships Initiative

Led training of **2000+ students** in scholarship preparation, coordinated IELTS training for **800+ candidates**, and built a mentoring network for **200+ students**.

1 JAN 2024 – 30 DEC 2024 Remote  
Head of PR – Undergraduate Research Initiative Al-Azhar Branch

Organized **30+ research sessions**, secured **20+ speakers**, and managed academic partnerships.

**CONFERENCES AND SEMINARS**

3 SEP 2023 – 5 SEP 2023 Cairo International Fair, Cairo, Egypt  
Pharmaconex 2023 Technical Conference | Pharmaconex | Attendee

20 AUG 2023 – 20 AUG 2023 Online  
Online Pharmaceutical Industry Event | Shortcut Team | Attendee

23 OCT 2023 – 23 OCT 2023 Al-Azhar Conference Hall, Cairo, Egypt  
The 7th Scientific Conference for EPSF | EPSF | Attendee

**LANGUAGE SKILLS**

Mother tongue(s): **ARABIC**  
Other language(s):

	UNDERSTANDING		SPEAKING		WRITING
	Listening	Reading	Spoken production	Spoken interaction	
ENGLISH	C1	C1	B2	B2	B2
DUTCH	A1	A1	A1	A1	A1

Levels: A1 and A2: Basic user; B1 and B2: Independent user; C1 and C2: Proficient user

**SKILLS**

Computational & Data Science

Python, Matplotlib, Seaborn, Scikit-learn

Cheminformatics & Molecular Modeling

Molecular docking (Gnina, Vina, MzDock) | RDKit, Mols2grid, Py3Dmol, SHAP | MD Simulations (GROMACS) | QM Simulaions (ORCA, Q-Chem)

## Experimental/Analytical Chemistry

Organic Synthesis | IR, NMR, UV-Vis | Antimicrobial analysis (IC<sub>50</sub>, MIC, FIC) | Melting point analysis | high-performance liquid chromatography | Electrochemical Characterization (CV, EIS, GCD) | Photoluminescence spectroscopy