

SHIVATMA RAI

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PROFESSIONAL SUMMARY

Computational Drug Discovery and Pharmacology professional with **7+ years of pharmaceutical industry experience**, an **M.Pharm in Pharmacology**, and a **PhD (Pursuing)** focused on Neurodegeneration. Experienced in molecular docking, structure-based drug design, protein and ligand preparation, protein–ligand interaction analysis, and **in silico** ADMET prediction using AutoDock Vina, PyMOL, BIOVIA Discovery Studio Visualizer, Meeko, and pkCSM. Strong background in scientific literature review, scientific writing, medical affairs, and evidence-based research. Passionate about applying computational approaches to accelerate early-stage drug discovery.

TECHNICAL SKILLS

Computational Drug Discovery

- Molecular Docking
- Structure-Based Drug Design (SBDD)
- Protein Preparation
- Ligand Preparation
- Protein–Ligand Interaction Analysis
- Binding Site Analysis
- ADMET Prediction
- Drug-likeness Assessment

Software & Databases

- AutoDock Vina
- AutoDockTools
- PyMOL
- BIOVIA Discovery Studio Visualizer
- Meeko
- pkCSM
- SwissADME
- PubChem
- RCSB Protein Data Bank

Research

- Scientific Literature Review
- Scientific Writing
- Research Methodology
- Pharmacology
- Evidence Synthesis

- Data Interpretation

RESEARCH PROJECT

In Silico Evaluation of Lawsone as a Potential Acetylcholinesterase Inhibitor

Techniques - AutoDock Vina • PyMOL • Discovery Studio • Meeko • pkCSM • SwissADME

Key Outcomes

- Performed protein preparation of human acetylcholinesterase (PDB ID: 4M0F).
- Prepared Lawsone and Donepezil ligands for molecular docking.
- Conducted molecular docking using AutoDock Vina 1.2.7.
- Obtained a best docking score of **-7.935 kcal/mol** for Lawsone.
- Compared docking performance with the reference inhibitor Donepezil (-11.41 kcal/mol).
- Performed protein–ligand interaction analysis using BIOVIA Discovery Studio Visualizer.
- Predicted ADMET properties using pkCSM.
- Authored a complete scientific manuscript based on the computational study.

EDUCATION

- PhD in Pharmacology (Pursuing) -Sanskriti University
-Research Area: Computational Drug Discovery for Neurodegenerative Disorders
- M.Pharm (Pharmacology)- RKDF University CGPA: 7.9
-Research: Antidepressant activity of Lawsonia inermis
- B.Pharm - Dr. A.P.J. Abdul Kalam Technical University

PROFESSIONAL EXPERIENCE

Assistant Scientific Manager

Avon Wellness | March 2026 – Present

- Conduct scientific literature reviews and evidence synthesis to support product development.
- Develop scientific documents, educational content, and CME materials for healthcare professionals.
- Collaborate with Regulatory Affairs, Medical Affairs, Product Management, and Marketing teams to ensure scientific accuracy and compliance.

Product Management & Medical Affairs

Unique Pharmaceuticals | July 2025 – March 2026 | Central African Republic

- Evaluated published scientific literature to support medical affairs initiatives.
- Developed evidence-based scientific communication materials and promotional literature.
- Managed product portfolios across cardiology, neurology, nephrology, gastroenterology, critical care, pain management, and orthopaedics.

- Supported healthcare professionals through scientific discussions and medical education activities.

Regional Manager

Alkem Laboratories | June 2024 – July 2025

- Interpreted clinical studies and pharmacological evidence for scientific communication.
- Developed scientific presentations and educational materials.
- Collaborated with Key Opinion Leaders (KOLs) and cross-functional teams to support scientific engagement.

Sales Officer – Scientific Liaison

Sun Pharmaceutical Industries Ltd. | January 2018 – June 2024

- Reviewed scientific literature and clinical publications to support evidence-based product communication.
- Developed product monographs, scientific presentations, and CME content.
- Conducted scientific discussions with healthcare professionals across multiple therapeutic areas.

PUBLICATION

Manuscript under preparation

"In Silico Evaluation of Lawsone as a Potential Acetylcholinesterase Inhibitor"

CERTIFICATIONS

- Clinical Data Management
- Clinical SAS
- Computational Drug Discovery
Molecular Docking
Self-directed research project

CORE STRENGTHS

- Computational Drug Discovery
- Molecular Docking
- Pharmacology
- Scientific Writing
- Medical Affairs
- Scientific Literature Review
- Protein–Ligand Interaction Analysis
- ADMET Prediction

