Parth Shahi

Ahmedabad, Gujarat, India • (+91) 910-411-0826
onemoleequals@gmail.com • linkedin

SUMMARY:

Enthusiastic Master of Science graduate in Organic Chemistry from Gujarat University, keen to transition into computational chemistry. Proficient in traditional organic chemistry techniques such as synthesis, characterization, and wet chemistry. Currently expanding expertise through coursework, including Harvard University's CS50x, gaining exposure to computer science fundamentals. Skilled in utilising software tools such as ChemDraw, AutoDock, MGLTools, ChimeraX, and Discovery Studio for molecular modelling and analysis. Actively participated in professional seminars and demonstrated dedication to continuous learning. Seeking opportunities to apply organic chemistry knowledge in computational research and contribute to advancements in drug discovery.

EDUCATION:

Gujarat University, School of Sciences, Department of Chemistry — Ahmedabad, India
Master of Science, Organic Chemistry — *May 2023*

- CGPA: 6.56/10, **First Class**
- Thesis: **"Molecular Docking Analysis of Biginelli Derivatives against BRAF Protein: A Study of Binding Affinities and Interactions"**
- Review paper (in review): **"A Comparative Study on the Synthesis of 5-Fluorooxindole via Various Pathways"**
- Participated in a variety of professional seminars and extracurriculars

Gujarat University, KKSJMSC — Ahmedabad, India
Bachelor of Science, Chemistry — *May 2021*

- CGPA: 6.92/10, **First Class** (top 5% in college)
- Graduated with high honours
- Volunteered under NSS for Medical Camp, Cleanliness Campaigns, etc.

GSEB, Hebron — Ahmedabad, India
5-12, Science with Mathematics (PCM) — *May 2018*

- Played for school football team in Inter-School Football tournament

CERTIFICATIONS:

Harvard University, CS50x — Remote
Introduction to Computer Science — *Ongoing, 75%*

- The 4-months entry-level course teaches students how to think algorithmically and solve problems efficiently.
- Topics include abstraction, algorithms, data structures, encapsulation, resource management, security, software engineering, and web development.

NIELIT, CCC — Remote
Course on Computer Concepts — *March 2019*

- 80-hours course that allows the students to get basic knowledge of computers.

SKILLS AND COMPETENCIES:

Core Competencies:

Critical thinking	Active learning	Team player
Problem solving	Literature	Research

Chemistry:

Synthesis	Data interpretation	Rotary Evaporator
GLP	Wet Chemistry	Sample Preparation
Routine TLC	Literature Search	Scientific Writing
Column Chromatography	Liquid-Liquid Extraction	

Softwares & Technologies:

ChemDraw	Discovery Studio	SciFinder
AutoDock	PyMOL	MestReNova
AutoDock Vina	Zotero	Microsoft 365
MGLTools	Bash	
ChimeraX	Linux	

Computer Languages:

C	HTML	JavaScript
Python	CSS	
SQL	Bootstrap	

Spoken Languages:

English (Fluent)	Hindi (Native)	Gujarati (Working Proficiency)

Interests & Activities:

Chess	Cycling
Football	Swimming

PROJECTS:

Thesis: "Molecular Docking Analysis of Biginelli Derivatives against BRAF Protein: A Study of Binding Affinities and Interactions"

Conducted a Master's dissertation under the guidance of Dr. Jayesh Maru, focusing on the computational analysis of 300 Biginelli derivatives against the BRAF protein, leveraging advanced techniques in molecular docking and computational chemistry.

Abstract: Investigated the potential of Biginelli derivatives as anti-cancer agents through molecular docking against the BRAF protein. Identified top ligands with superior binding affinities, showcasing their promise for targeted cancer therapy.

Research Methodologies:

- Utilised Chemdraw and Open Babel for the preparation of 300 ligand molecules.
- Employed UCSF ChimeraX, Autodock, and Autodock Vina for the rigorous cleaning, preparation, and blind docking of BRAF protein against ligands.

Analysis Tools:

- Applied PyMOL and Discovery Studio Visualizer for 3D and 2D visualisation and analysis of docking results.

Results and Achievements:

- Identified 62 ligands surpassing the binding affinities of standard co-crystallized ligands.
- Top 10 ligands, particularly urea and methyl urea substituted, demonstrated strong potential as BRAF inhibitors.

Conclusion: Concluded that Biginelli derivatives exhibit significant promise as BRAF inhibitors, offering valuable insights for further experimental studies in cancer treatment.

Skills Developed:

- Proficient in molecular docking using Autodock Vina.
- Expertise in computational chemistry techniques for ligand and protein preparation.
- Skilled in 3D and 2D visualisation using PyMOL and Discovery Studio.

Review Paper: "A Comparative Study on the Synthesis of 5-Fluorooxindole via Various Pathways"

Authored a review paper under the guidance of Dr. Jayesh Maru on the synthesis of 5-Fluorooxindole, a pivotal intermediate in sunitinib production for treating renal cell carcinoma and gastrointestinal stromal tumours.

Abstract: Explored diverse synthesis methods for 5-Fluorooxindole, essential in sunitinib production. This review provides a concise overview of pathways, including Wolff-Kishner reduction and metal-catalysed reactions, emphasising the compound's significance in commercial drug synthesis.

Key Insights:

- Various synthesis methods: Wolff-Kishner reduction, Friedel-Crafts alkylation, metal and clay catalysed reactions.
- Crucial role of 5-Fluorooxindole as a sunitinib intermediate.

Conclusion: The review concludes that efficient 5-Fluorooxindole synthesis is vital for sunitinib production. While the low-valent titanium method is fastest, the 5-fluoro-3-methylthio-2-oxindole method yields maximum efficiency. Ongoing research aims for more cost-effective synthesis.

REFERENCES:

Dr. Jayesh J. Maru
(Thesis Guide)
Asst. Professor
Dept. of Chemistry, School of Sciences, GU
Email: jaymaru@gujaratuniversity.ac.in