

Vilnius University – Institute of Data Science and Digital Technologies

Glauco Endrigo **PhD Student**

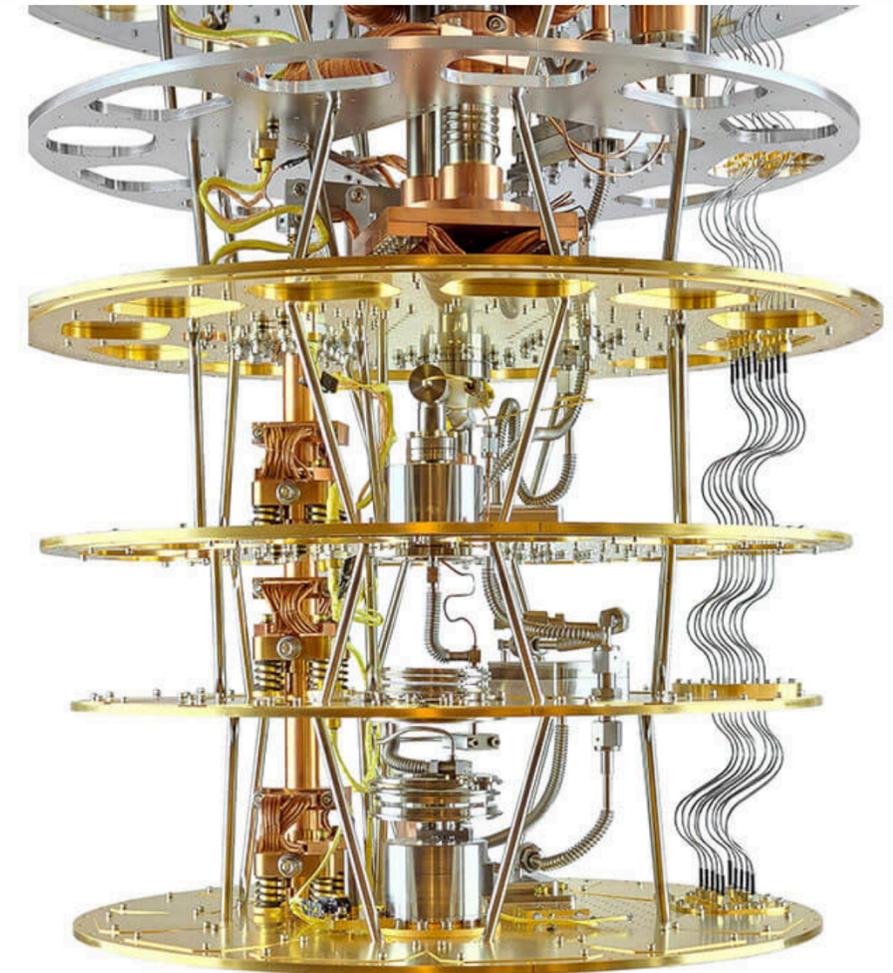
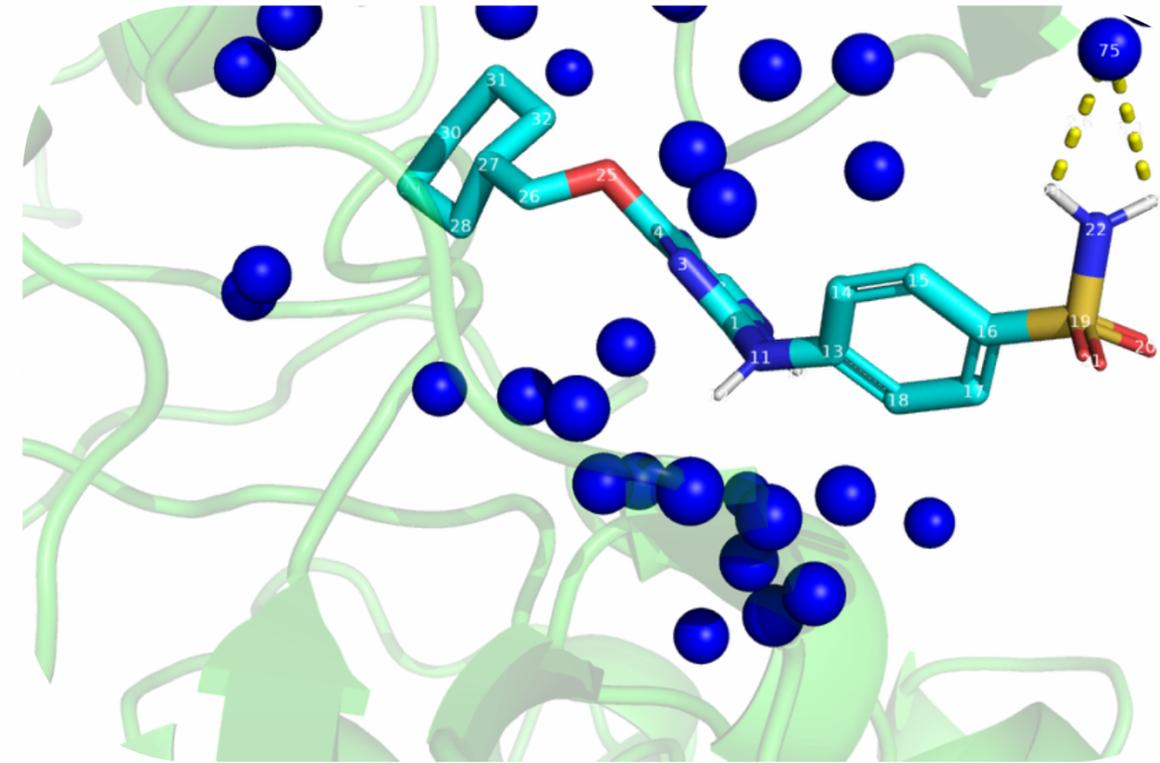
- Dissertation Title: Novel Quantum Representations of Molecular Systems for Quantum Generative Models
- Studies Period: 1 October 2025 – 30 September 2029
- Current Year of Study: Year 1
- Faculty of mathematics and informatics
- Informatics n009

Supervisor: Dr. Remigijus Paulavičius

The research **goal** **and motivation**

Design and implement a **novel quantum encoding of molecular systems**, specifically tailored and optimised for integration with **quantum machine learning (QML)**.

- These representations are intended to enhance the expressive capacity, noise tolerance, entanglement utilisation, and overall resource efficiency of quantum machine learning



Summary of the **plan of study**

Study Years	Exams ¹	
	Planned	Completed
I (2025/2026)	2	1
II (2026/2027)	2	0
III (2027/2028)	0	0
IV (2028/2029)	0	0
Total:	4	1

Study Years	Conference Participation				Publications					
	International ²		National ³		With Impact Factor ⁴			Without Impact Factor ⁵		
	Plan	Done	Plan	Done	Plan	Done ⁶	Status ⁷	Plan	Done ⁶	Status ⁷
I (2025/2026)	0	0	1	0	0	0	-	0	0	-
II (2026/2027)	1	0	0	0	1	0	-	0	0	-
III (2027/2028)	1	0	0	0	1	0	-	0	0	-
IV (2028/2029)	0	0	0	0	0	0	-	0	0	-
Total:	2	0	1	0	2	0		0	0	

Exams 2025/2026 (Semester I)		
Plan	Completed	Status
Machine Learning (2026 y. I quarter)	Machine Learning (2026 y. I quarter)	Passed

Summary of the **plan of study**

No.	Publication's title	Fulfilment period		Notes
		From	To	
1.	Review and analysis of scientific research related with the theme of doctoral thesis (in Lithuania and abroad):			
1.1.	Quantum Computing Fundamentals: Grasping quantum principles (superposition, entanglement), essential algorithms, and familiarizing with quantum hardware (superconducting qubits, trapped ions, annealers)	2025 y. IV quarter	2026 y. I quarter	Done
1.2.	Focused Literature Review: Core Methodologies Conducting a comprehensive review of Quantum Generative Models (e.g., GANS, Diffusion Models, VAEs) and advanced molecular encoding strategies to identify key opportunities.	2025 y. IV quarter	2026 y. I quarter	A review paper has been drafted and is presently in the final revision stage with the supervisor; it is nearing the formal submission process

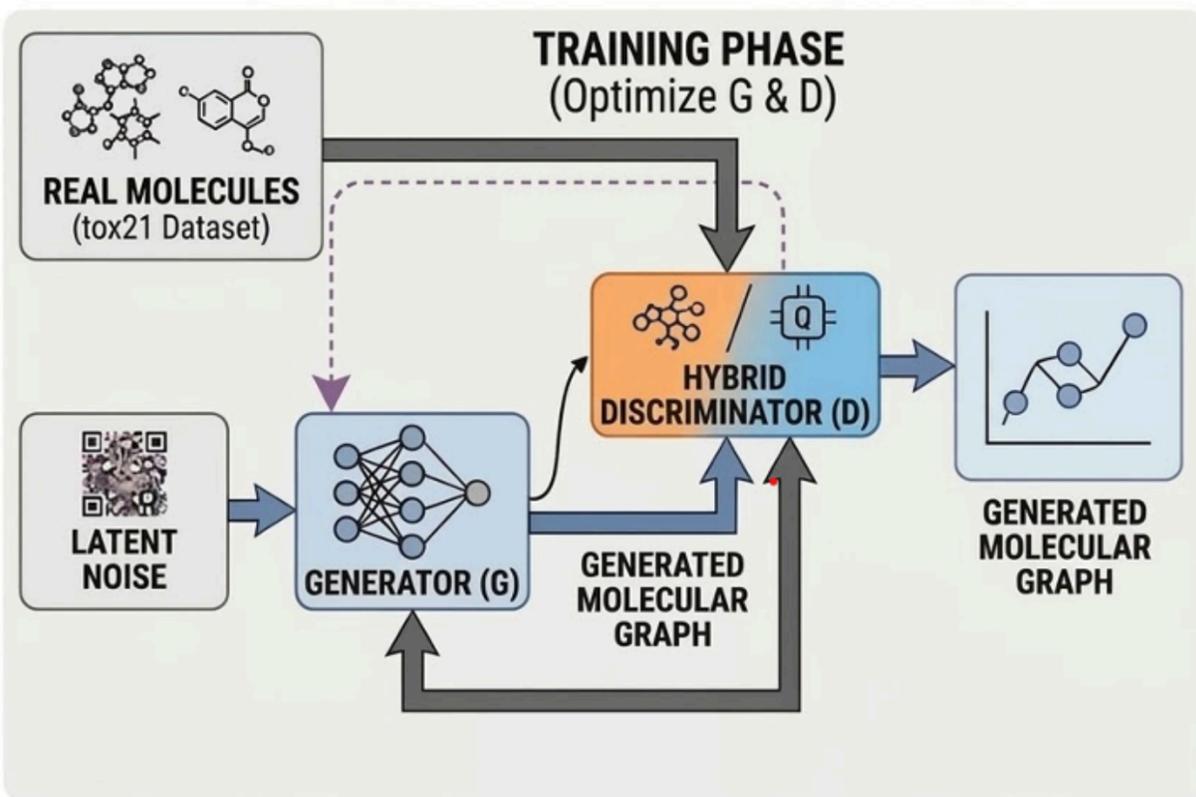
Summary of the **plan of study**

No.	Publication's title	Fulfilment period		Notes
		From	To	
1.3.	Problem Formulation: Phase 1 Generate a portfolio of radical hypotheses by mining analogies from out of the box paper in the field.	2026 y. I quarter	2026 y. II quarter	A foundational framework integrating Generative Adversarial Networks (GANs) and hybrid quantum-classical networks has been established based on the literature, thereby facilitating comprehensive empirical validation in subsequent research stages. Crucially, the systematic identification of existing research gaps and limitations within the field has provided a robust basis for the formulation of a rigorous research hypothesis. To date, all project milestones have been successfully achieved; consequently, current efforts are focused on the problem formulation phase, in strict accordance with the established research plan.

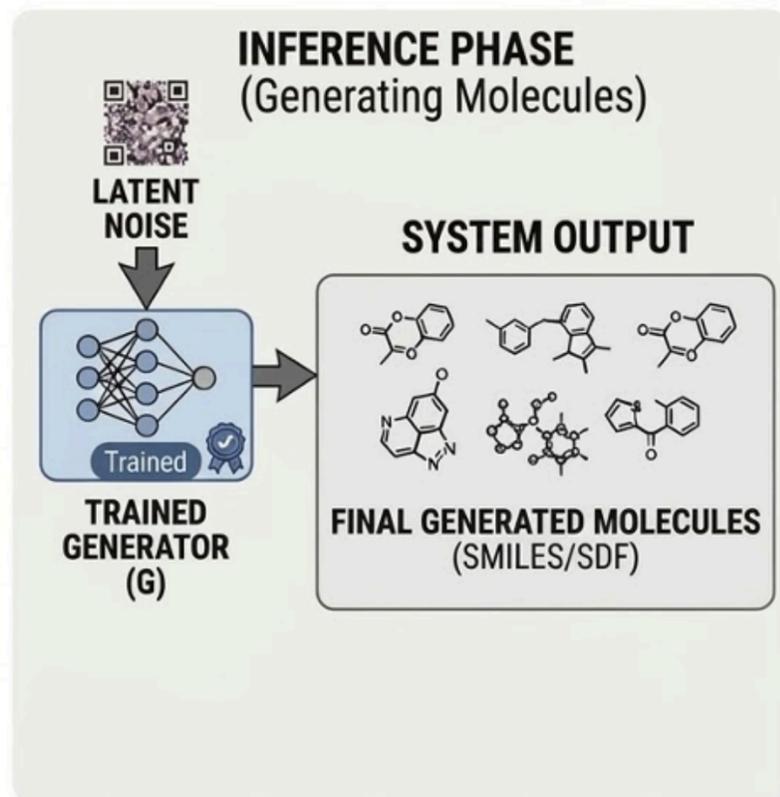
State of the Art Review

- Discriminative, generative, and optimization-based quantum models
- Quantum molecular representations strategies.
- Hybrid quantum-classical strategies to bypass hardware limitations like noise, limited qubit counts, and barren plateaus .
- Platforms and constraints
- Future directions

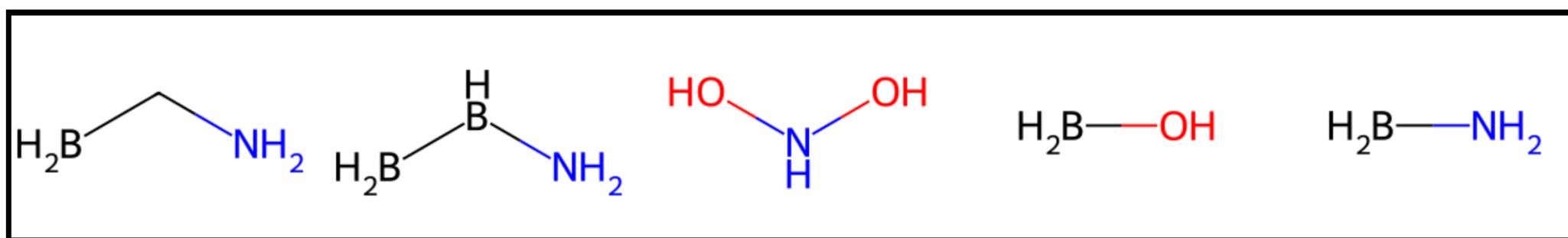
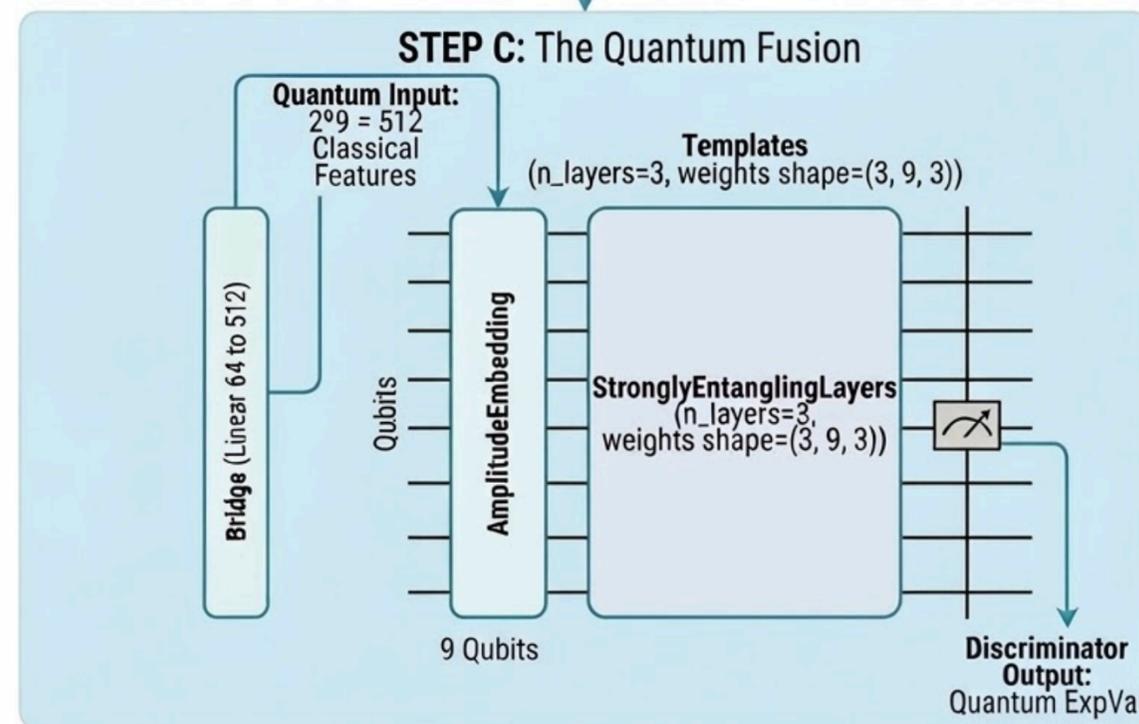
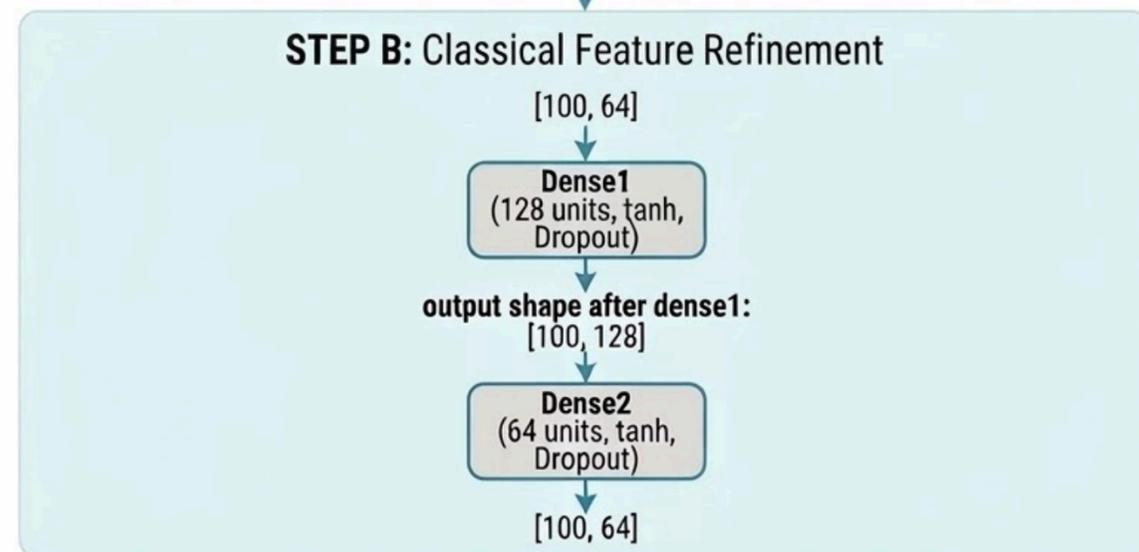
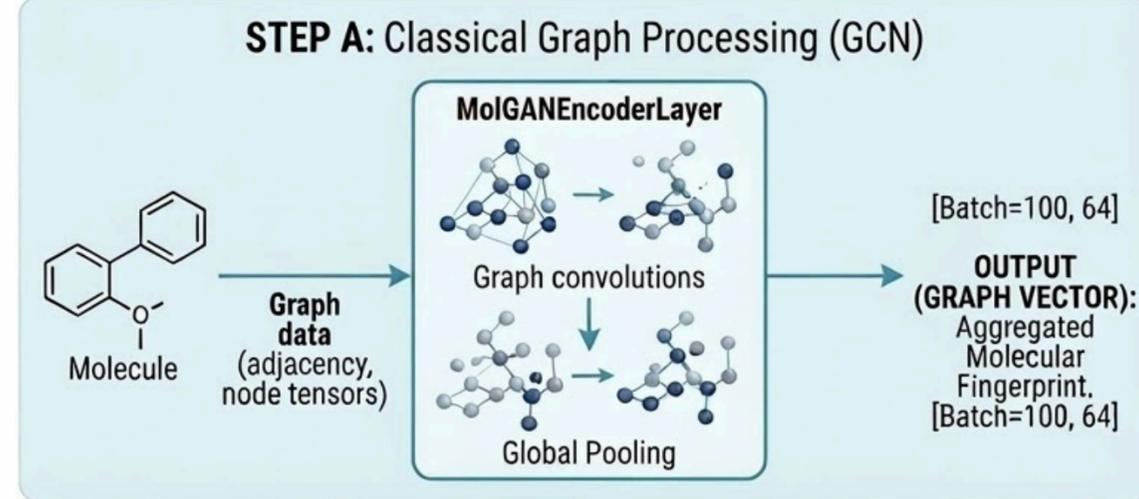
Scientific results



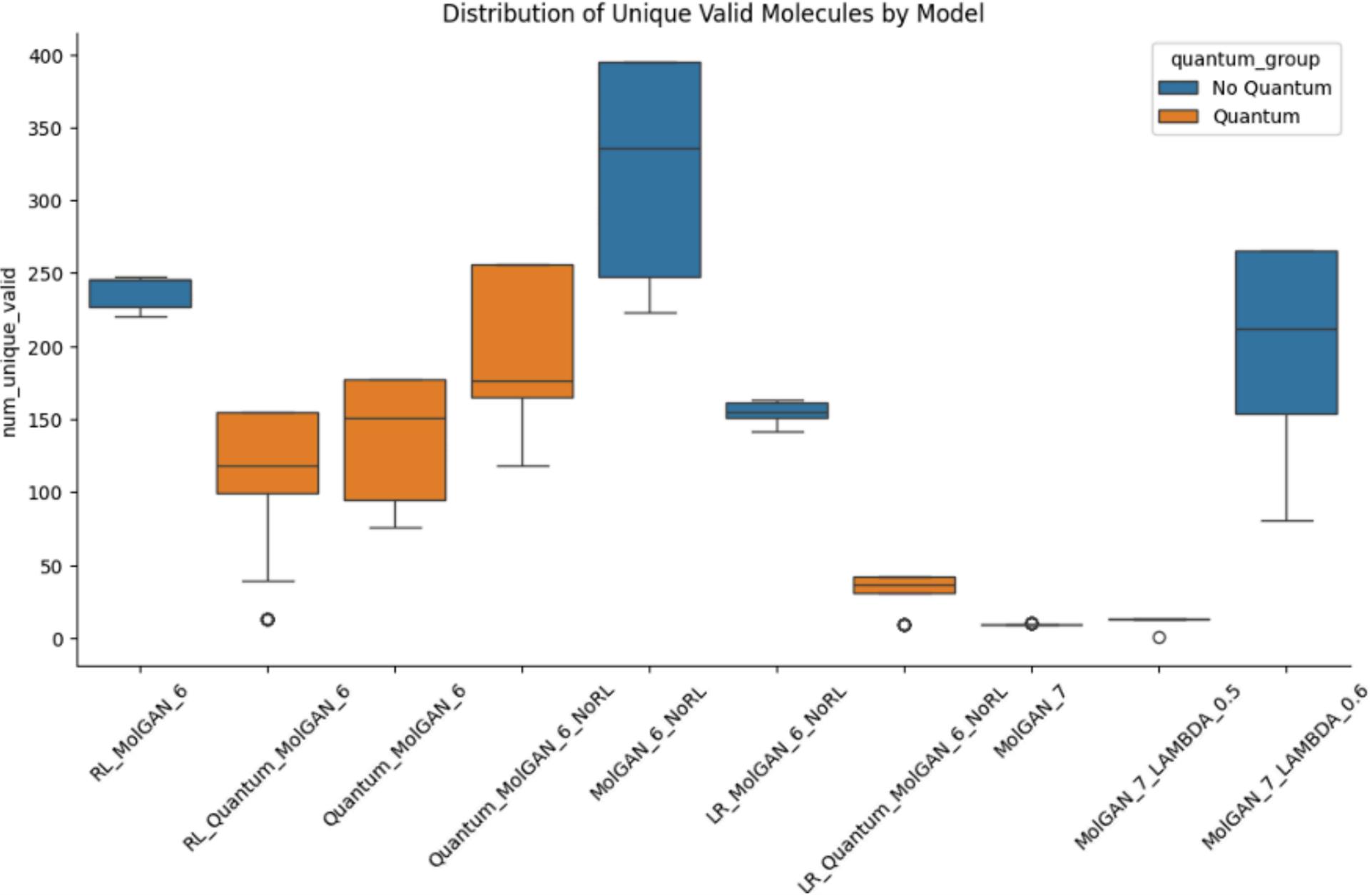
TRAINING PHASE
(Optimize G, D & D)



INFERENCE PHASE
(Generating Molecules)



Scientific results



Work plan for the next semester.

- Phase 1 (2026, I–II quarter): Generate a portfolio of radical hypotheses by mining analogies from out of the box papers in the field.
- Phase 2 (2026, II–III quarter): Kill bad ideas fast. Subject top hypotheses to time-boxed validation tests using toy model simulations and pre-defined performance metrics.
- Phase 3 (2026, IV quarter): Synthesize sprint results into a single, validated research problem with a clear roadmap and risk assessment

4^o Quarter of 2026:

- Present research results at a national scientific conference.
- Participate in an international summer/winter school for PhD students

Acknowledgments and Q&A

“Hinc itur ad astra”