

Vilnius University – Institute of Data Science and Digital Technologies

Glauco Endrigo

Semester II

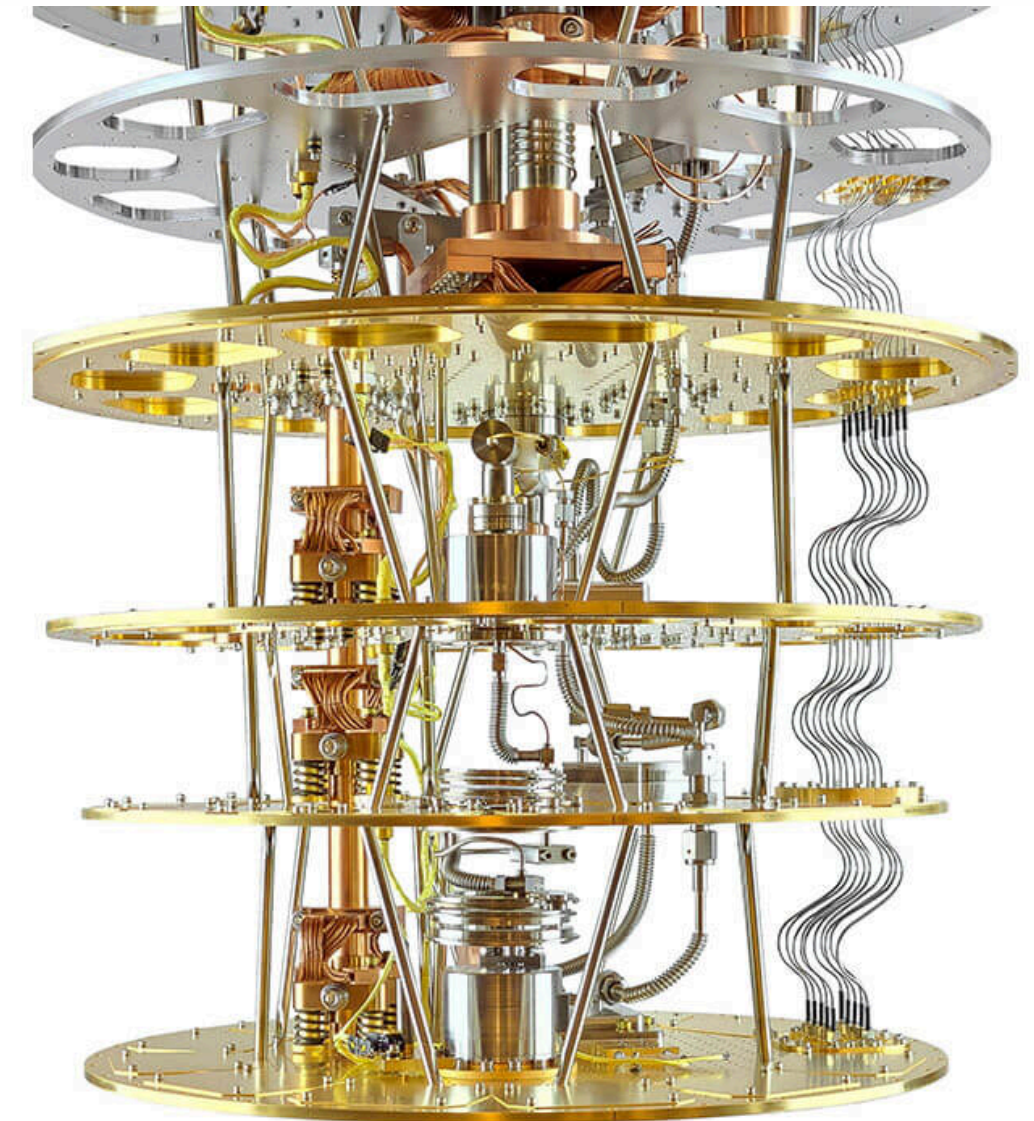
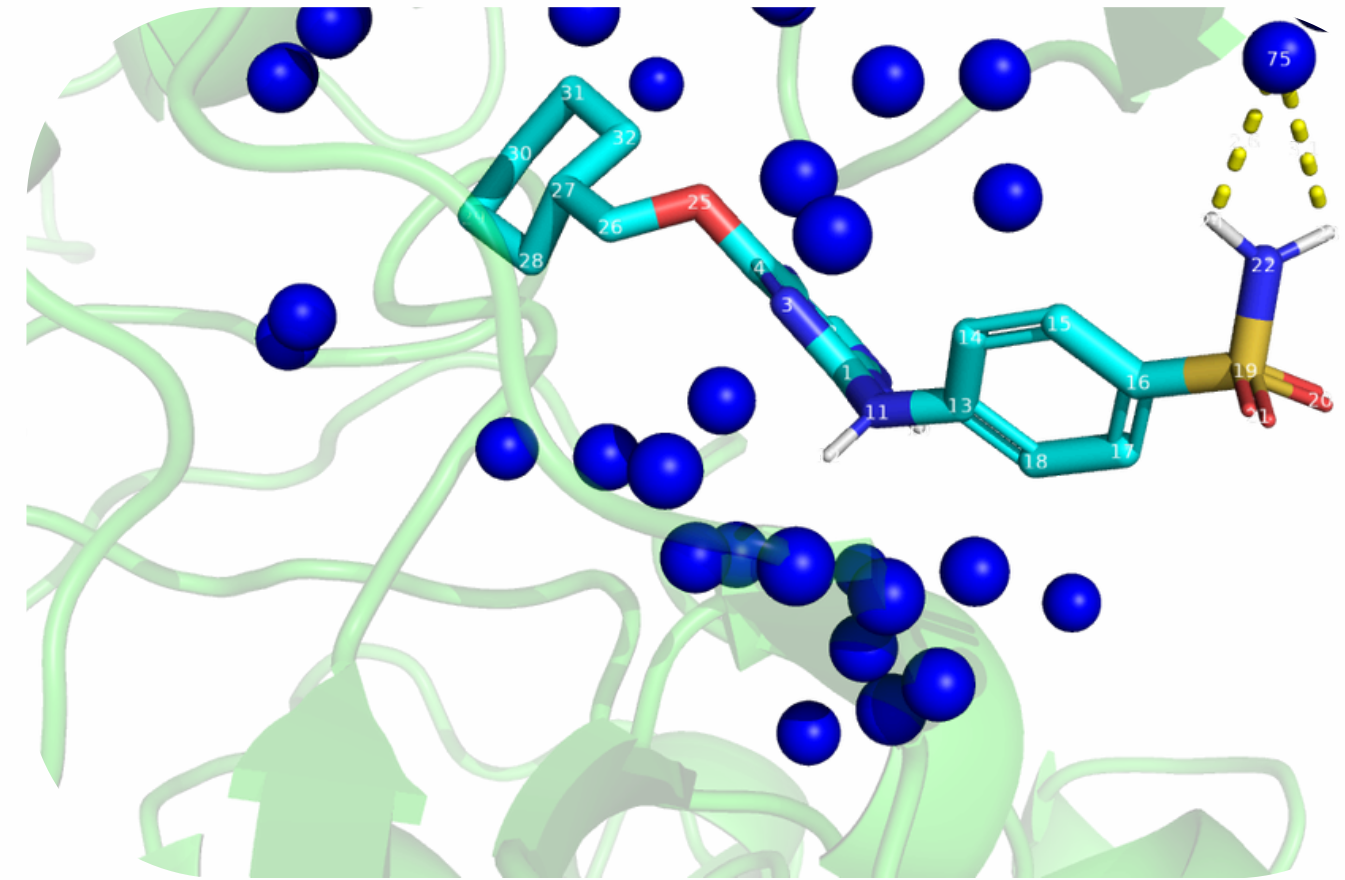
- Reporting period: April–September 2026
- Dissertation: Novel Quantum Representations of Molecular Systems for Quantum Generative Models
- Informatics (N009) · Faculty of Mathematics and Informatics

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 2025/2026 to 2028/2029

Study year	Planned milestones	Completed so far
I (2025/2026)	2 exams	2 exams; 2 summer/winter schools
II (2026/2027)	2 exams; 1 national conference; 1 summer school	—
III (2027/2028)	1 international conference; 1 school; 1 research mobility; 1 impact-factor paper	—
IV (2028/2029)	1 international conference; 1 impact-factor paper	—

Summary of the plan of study

No.	Plan	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	Semester II update: Pursued the exploratory objective of Plan item 1.3 by drawing on ideas from graph diffusion to investigate photonic representations for molecular generation. This led to a testable research question on how representation choices affect prediction sensitivity and generative performance, and to the definition of a controlled comparison with classical models. Exploratory tests were also conducted on the physical ORCA PT-1 photonic quantum computer, accessed through the Poznań Supercomputing and Networking Center (PSNC).

Summary of the plan of study

No.	Plan	Fulfilment period		Notes
		From	To	
1.4.	Problem Formulation: Phase 2 - Kill bad ideas fast. Subject top hypotheses to time-boxed validation tests using toy model simulations and pre-defined performance metrics.	2026 y. II quarter	2026 y. III quarter	Semester II update: Pursued the validation objective of Plan item 1.4 through simulations and quantitative evaluation of candidate photonic designs. Developed and implemented a mathematical framework connecting photonic state geometry, information accessible through measurement and molecular prediction sensitivity. Formulated geometric criteria for selecting circuit architectures and control placements. Calibrated classical reference models and determined their control dimensions by matching task-Fisher spectral summaries. Conducted a controlled comparison of photonic and classical molecular generation under common data, training and sampling conditions. Tests on the physical ORCA PT-1 photonic quantum computer were also carried out during this phase, alongside the simulation-based evaluation.

Year I record through Semester II

EXAMS

- Machine Learning
- Research Methods in Informatics and Informatics Engineering

SUMMER / WINTER SCHOOLS

- WISER Summer Program | 8 June–31 July
- Qiskit Global Summer School | 13–24 July

CONFERENCES

- Build Stuff 2026 | 2–4 Dec Vilnius | Accepted speaker
- DAMSS 2026 | 26–28 November, Druskininkai | National (planned)

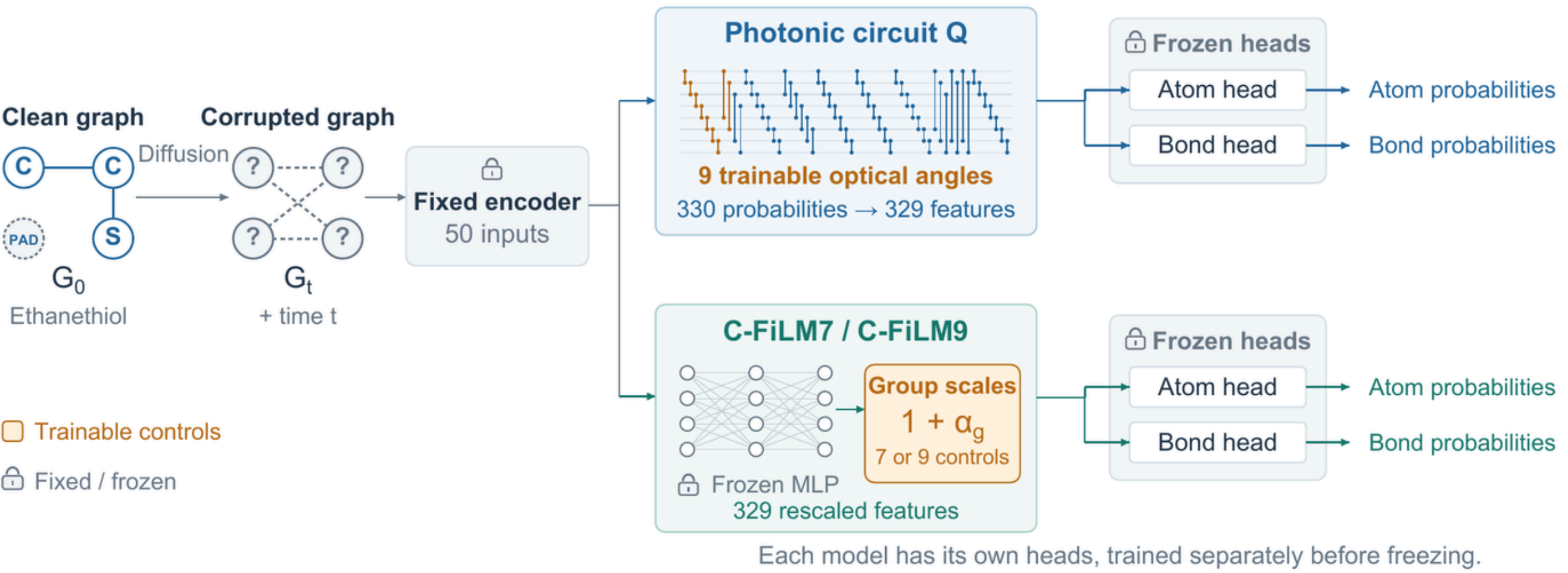
Additional Activities

- 29 Oct · Tyrėjų Grand Prix final, Vilnius — Qualified to final

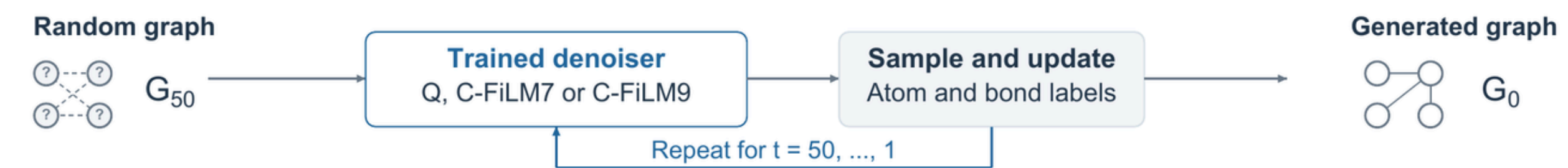
Scientific results: Controlled molecular generation

a Photonic and classical denoisers

Control-training stage: the feature controls change; prediction-head weights do not.



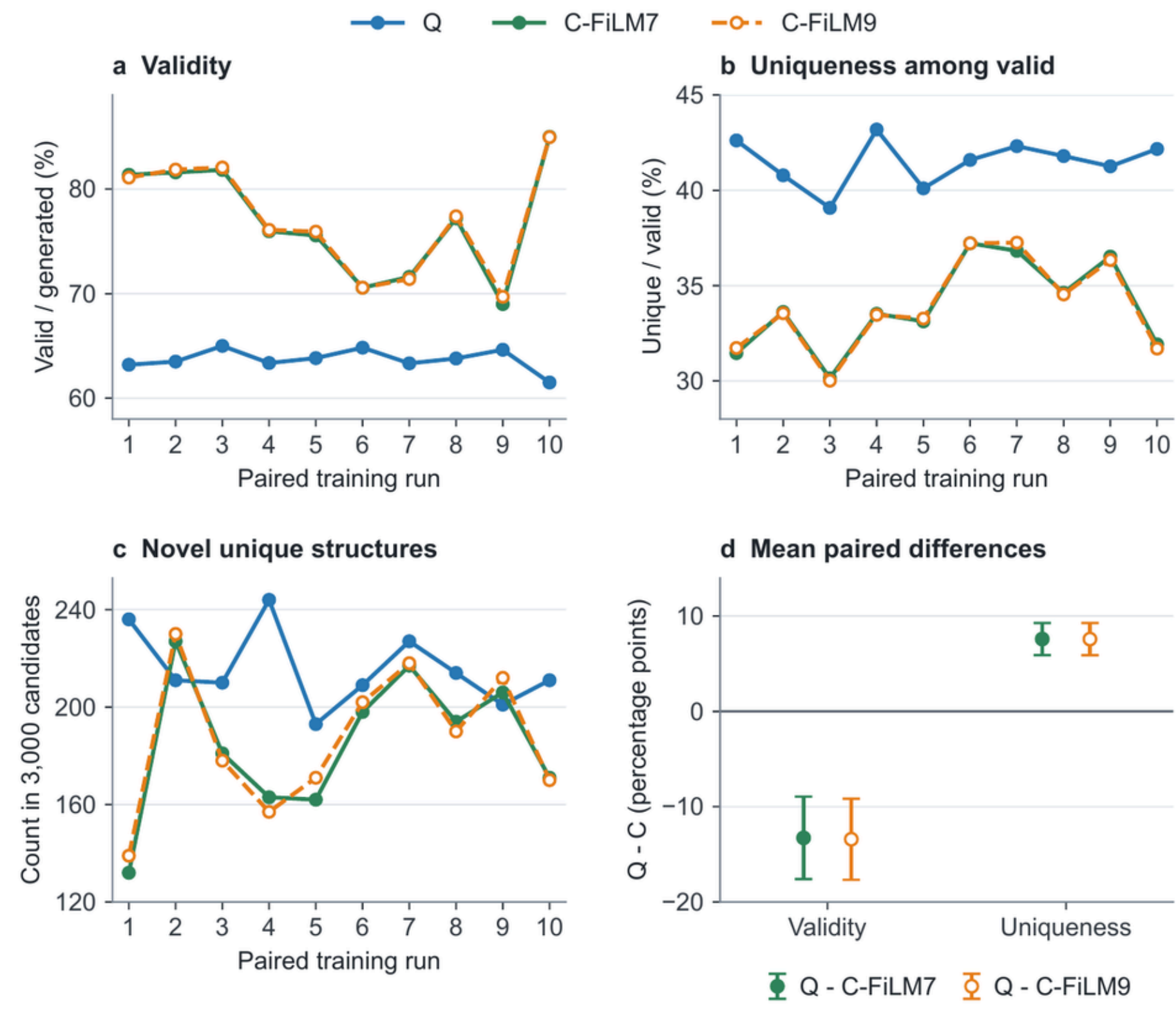
b Reverse diffusion for molecular generation



Controlled comparison

- 01** The same graph and diffusion step enter each denoiser.
- 02** Photonic and classical models have separately trained heads.
- 03** Reverse diffusion samples each trained model independently.

Scientific results Validity–diversity trade-off



Measured trade-off

Lower validity

Q generated fewer valid structures in all 10 paired runs.

Higher uniqueness

Among valid outputs, Q was more diverse in all 10 runs.

More novel unique structures

Q exceeded C-FiLM7 in 8 of 10 paired runs.

Higher diversity comes with lower validity; no overall quantum advantage is claimed.

Work plan for the next semester.

- Phase 3 (2026 y. IV quarter–2027 y. I quarter): Consolidate the findings into a validated research problem: how to improve molecular validity while preserving diversity. Define a clear roadmap and risk assessment.

Molecular encoding (begins 2027 y. I quarter): Explore new ways to encode molecules on quantum computers for quantum machine learning, using parts of the mathematical framework developed so far to show their benefits. If feasible, investigate whether a molecule's quantum information can be encoded directly in a quantum computer without loss, and use the framework to demonstrate the benefit of doing so.

Also planned:

- DAMSS 2026: participation and abstract submission planned (26–28 November, Druskininkai).
- Fundamental Methods of Informatics and Informatics Engineering Science exam.

Acknowledgments and Q&A

“Hinc itur ad astra”