Computer-assisted drug design with latent style-based quantum generative modelling

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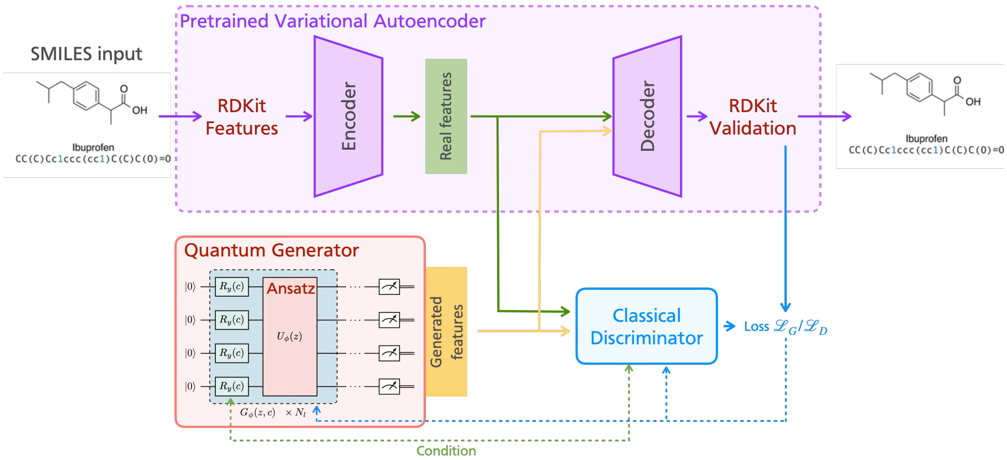
ABSTRACT

Pharmaceutical development is a tedious, time-consuming, and expansive process up to a mean expense around $2.5 billion. In the entire drug development pipeline, the first step is the design of new molecular structures. Such de-novo design assisted by artificial intelligence (AI) has expanded significantly in the past few years, and generative AI has delivered promising results in creating new molecular structures compatible with targeted criteria [1], reducing costs and time to solution. Generative adversarial networks (GANs) are in particular used for de-novo drug design, but they are difficult to train and subject to mode collapse. Using quantum computing may overcome these issues and we propose a new hybrid style-based quantum GAN (QGAN) architecture [2] for computer-assisted drug design [3], using a latent-space encoding of the molecules via a variational autoencoder, a classical discriminator, and a quantum generator. The vectors from the latent space are the input of the quantum generator of the QGAN:



We will present our baseline model with gradient penalty to mitigate mode collapse and a Wasserstein distance for the training. Our architecture is validated on quantum simulators with 10 qubits and we present inference runs on an IBM Heron quantum computer using 5 qubits and dual readout. We benchmark our results against classical models as provided by the industry-relevant MOSES benchmark suite [4]. Our QGAN obtains competitive results in terms of validity, uniqueness, internal diversity, or LogP, using far less trainable parameters compared to a classical GAN.

[1] Xiangru Tang, Howard Dai, Elizabeth Knight, Fang Wu, Yunyang Li, Tianxiao Li, and Mark Gerstein. "A survey of generative AI for de novo drug design: new frontiers in molecule and protein generation". Briefings in Bioinformatics **25**, bbae338 (2024).

[2] Carlos Bravo-Prieto, Julien Baglio, Marco Cè, Anthony Francis, Dorota M. Grabowska, and Stefano Carrazza. "Style-based quantum generative adversarial networks for Monte Carlo events". Quantum **6**, 777 (2022).

[3] Julien Baglio, Yacine Haddad, and Richard Polifka. "Style-based Quantum Wasserstein GAN for Drug Design" (2026). To appear.

[4] Daniil Polykovskiy *et al.* "Molecular Sets (MOSES): A Benchmarking Platform for Molecular Generation Models" (2020) arXiv:1811.12823. arXiv:1811.12823 [cs].