Applied Quantum Computing

BIN Packing and Tumour Inhibiting Molecules
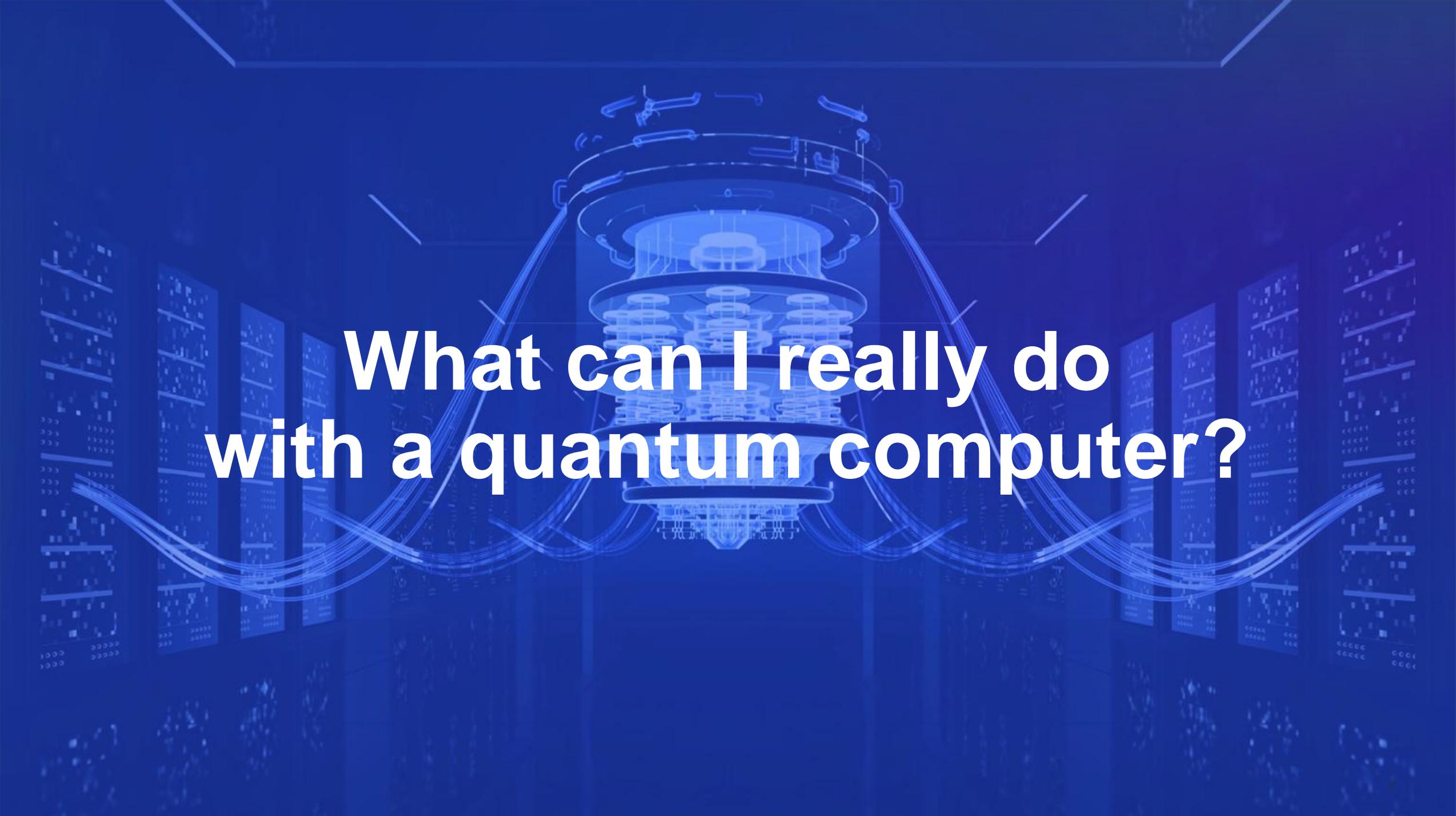
What can I really do with a quantum computer?

How is this relevant
to my business?

Optimization

The X% Edge

Molecule

Synthesis

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Our Speakers

Daniel Guisado

IT Manager & Information Security Officer

WÜRTH

Alma María Ortuño

Applied Quantum Specialist

Telefónica

Irene Lopez de Vallejo

Head of Q-Tech Business Development

tecnalia
MEMBER OF BASQUE RESEARCH & TECHNOLOGY ALLIANCE

Boosting Logistics operations Efficiency
With Quantum Computing in Würth scenario
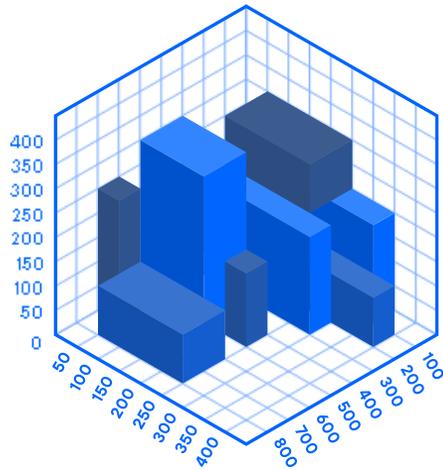
3D Bin Packing
Q-Algorithm

- Hybrid Algorithm on Dwave
- Tecnalia Solver
- Qcentroid Quantum Framework

FASTER

LOWER COST

BETTER VOLUME

BETTER NUM ITEMS

BETTER WEIGHT

BETTER NUM BINS
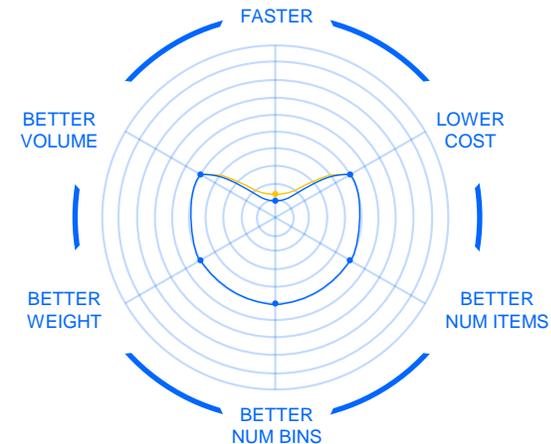
Quantum Metrics
and Benchmarking

- Quantum Performing Metrics
- Comparison with Classic 3D Bin Packing Model
- 30% Optimized orders forecasted

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Quantum 3D
Bin Packing

Optimize Space, reducing number of containers, shipping costs by faster and more sustainable operations

01.

Faster

Acceleration thanks to Hybrid Solver on D-Wave Quantum Computer

02.

Lean Operations

Better Packaging Process thanks to the new hybrid 3D Bin Packing powered by Quantum Computing

03.

Lean Operations

More scale: more packages and more business' rules resolved in each solver execution to achieve more productivity

04.

Lower Energy Footprint

Shorter executions on efficient hardware will reduce energy consumption

05.

Quantum Evolution

Solvers prepared to run on future, more powerful quantum computers

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Our Speakers

Jorge Andrés Plazas

Professor and Researcher

UFV Universidad Francisco de Vitoria

Angel Ayuso

Executive & Scientific Director

vithas
vivir para cuidarte

Juan Cumbrado

Applied Quantum Specialist

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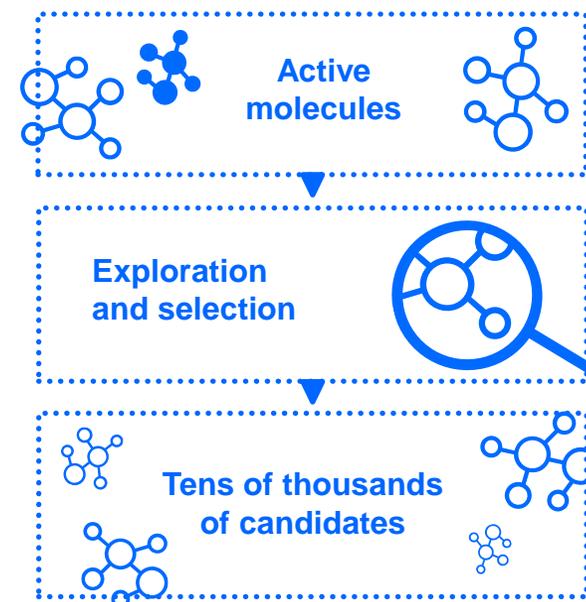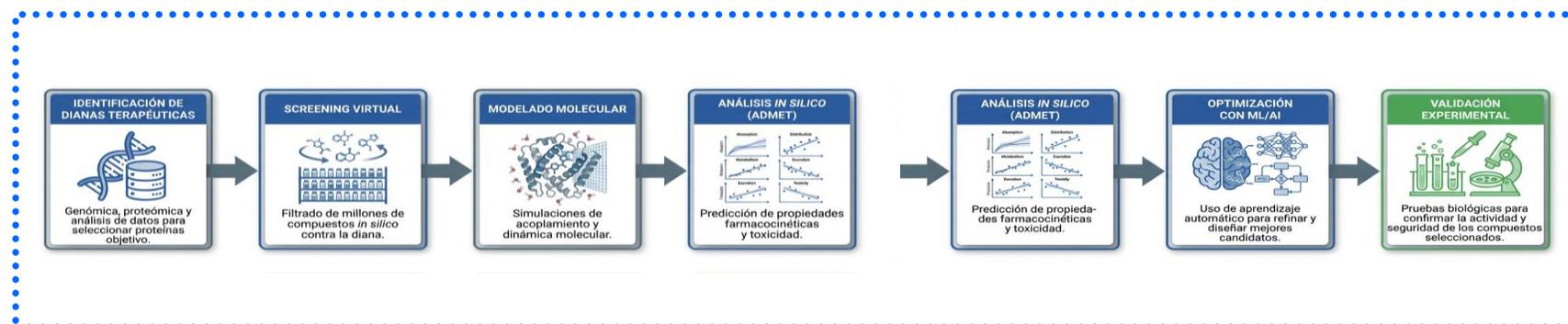
Name Surname

Applied Quantum Specialist

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Novel drug
discovery process
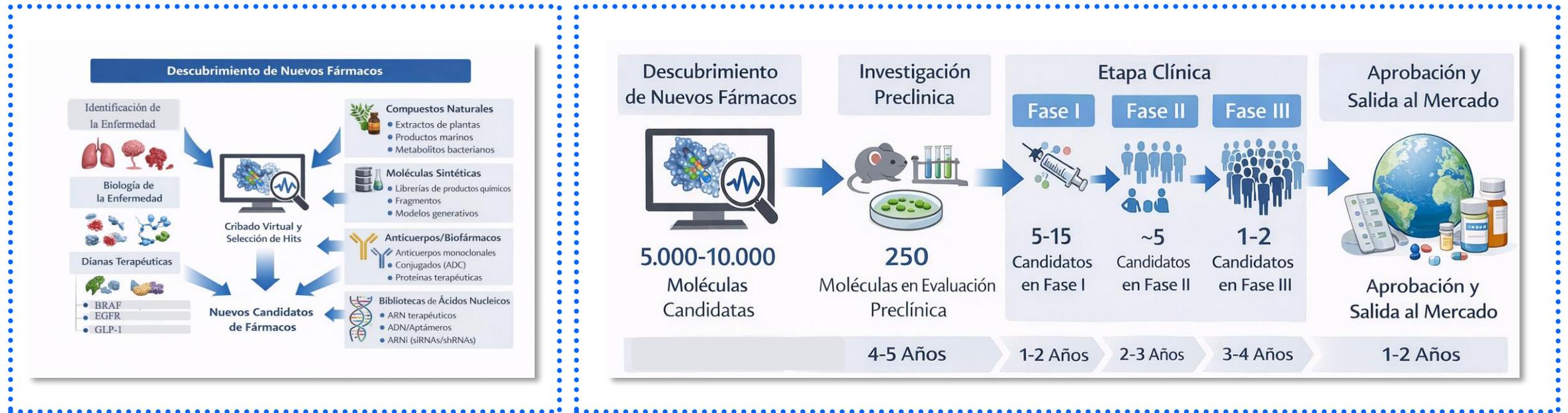
Drug reposition and discovery
using computational methods (In silico)

IDENTIFICACIÓN DE DIANAS TERAPÉUTICAS

Genómica, proteómica y análisis de datos para seleccionar proteínas objetivo.

SCREENING VIRTUAL

Filtrado de millones de compuestos *in silico* contra la diana.

MODELADO MOLECULAR

Simulaciones de acoplamiento y dinámica molecular.

ANÁLISIS *IN SILICO* (ADMET)

Predicción de propiedades farmacocinéticas y toxicidad.

ANÁLISIS *IN SILICO* (ADMET)

Predicción de propieda-des farmacocinéticas y toxicidad.

OPTIMIZACIÓN CON ML/AI

Uso de aprendizaje automático para refinar y diseñar mejores candidatos.

VALIDACIÓN EXPERIMENTAL

Pruebas biológicas para confirmar la actividad y seguridad de los compuestos seleccionados.

Computational search across the space of potential chemical structures to identify a manageable number of "virtual hits" that can be synthesized and experimentally tested in the laboratory
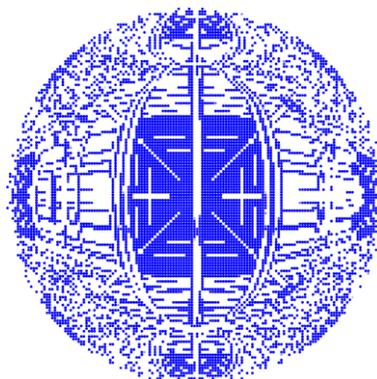
▶ **Shorter development time**

▶ **Lower investment**

Active molecules

Exploration and selection

Tens of thousands of candidates

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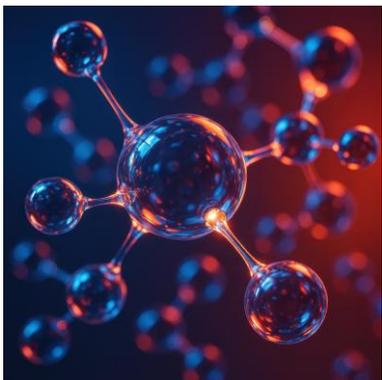
Exploration of Chemical Space I

Small number of known inhibitors used as a starting point (approx. 10^2).

Exploration of Chemical Space II

Through mutations, new molecules are generated, expanding the training dataset for the models (approx. 10^5).

Exploration of Chemical Space III

Structural property analysis using machine learning models.

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Generative models

Machine learning is used to learn the distribution of molecules in chemical space and enable the generation of new molecules.

Hybrid models with quantum components

The high structural complexity of the data distribution creates the need for new techniques.

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01.

Initial molecules

Tested inhibitor molecules used for learning.

02.

Neural network

Long Short-Term Memory (LSTM) neural network.
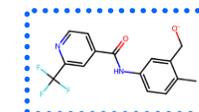
Learns molecular grammar.

03.

Quantum model

Quantum Circuit Born Machine (QCBM).

Finds complex patterns to guide the generation.

04.

Molecule generation

Creation of new molecules following learned rules.

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How does the quantum
part help?

Classical Approach

Good at producing valid molecules

Relies on simple or random starting points

May overlook complex feature combinations

Quantum Advantage

Starts from a learned, structured distribution

Captures complex correlation patterns

Improves diversity and quality of candidates

Quantum computing enables richer exploration of molecular possibilities

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Results
& Demo

Generative vs
Original Molecules

QED

+77% Drug-likeness

SA

+25% Synthetic
Accessibility

SA

+77% Drug-likeness

Simulation settings

Define the quantum circuit (VQC) parameters and the reward
optiimization strategy

QUANTUM MODEL

Number of Qubits

8 Qubits

Molecules to generate   100

EXECUTION ENVIRONMENT

Simulator   Real QPU

REWARD STRATEGY

Priority: Docking
D:0.6 | Q:0.3 | N:0.1

Priority: QED

Priority: Innovation

Start generation ▶

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