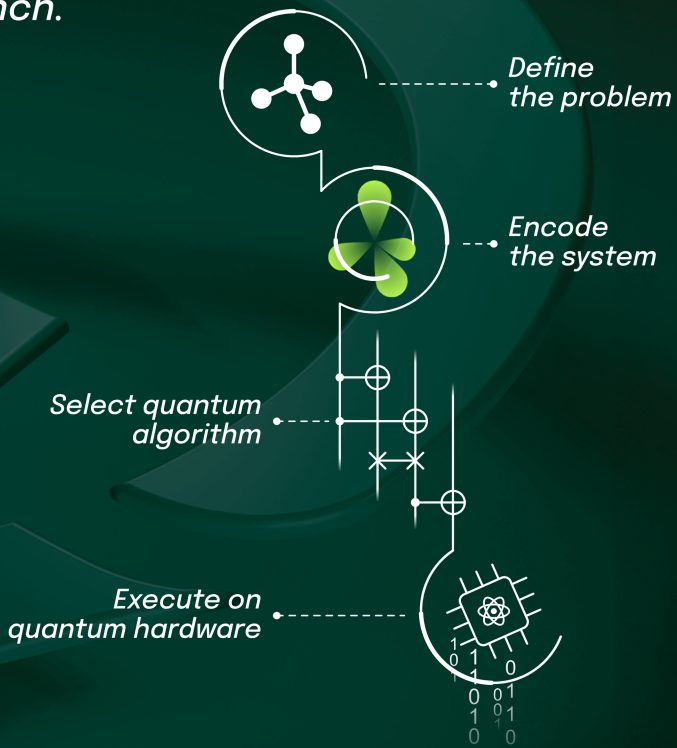
Quantum computing for life sciences should be easy

kvantify qrunch

- that's why we have developed Kvantify Qrunch.

- **Qrunch** is built for chemists. It is the easiest way to adopt quantum computing and do advanced chemistry computations on real quantum hardware.
- **Qrunch** enables full exploitation of quantum computing hardware for large-scale molecular simulations.
- **Qrunch** delivers the leap in performance needed to pioneer real-world applications – already today.



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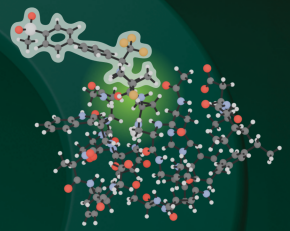
Kvantify Qrunch showcases

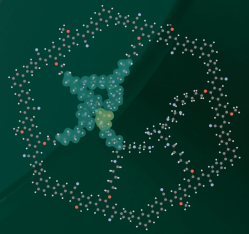
Scaling Covalent Ligand Simulations

The odanacatib ligand is a potent and highly selective covalent inhibitor of the Cathepsin-K enzyme, associated with osteoporosis. Using Qrunch with our BEAST-VQE algorithm, we simulated this covalent ligand binding on Rigetti's Ankaa 3 device. Using 80-qubits we executed a quantum algorithm embedded in a GPU accelerated DFT calculation. An exact simulation on classical computers is infeasible, and even approximations are very demanding.



Direct Air Carbon Capture

COF-999 shows enhanced CO2 uptake in humid conditions and is a promising material for direct air carbon capture. We simulated how a water molecule influenced the transition state energies of CO2 binding reactions in COF-999 using Qrunch. Using IQM's quantum hardware, we showed that our algorithms rapidly converged towards the ideal scenario despite the noisy backend.



Simulating Battery Chemistry

Butyronitrile is a promising electrolyte candidate in advanced technologies such as lithium-ion batteries and dye-sensitized solar cells (DSSC). With Qrunch we performed simulations of Butyronitrile dissociation on IQM Emerald. Our algorithms used all 54 qubits efficiently thanks to our gate compilation and optimization. Our result is beyond the reach of exact classical methods.