kvantify

Quantum Computing for Drug Discovery

Building the Path to Practical Applications

Patrick Ettenhuber | Quantum Innovation Manager | Kvantify

AIDDD 2026 | Boston | 27 October 2026

Classical ranking of protein-ligand interactions by k_{off} rate prediction enabled by force fields.

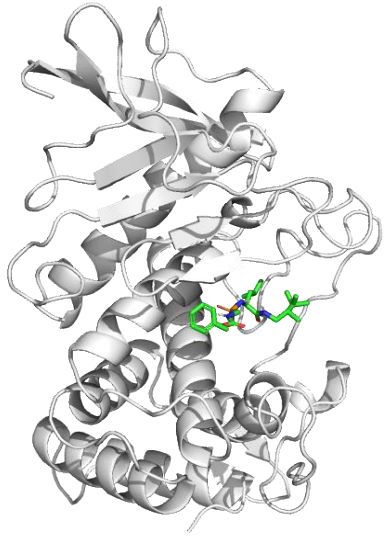
kvantify koffee

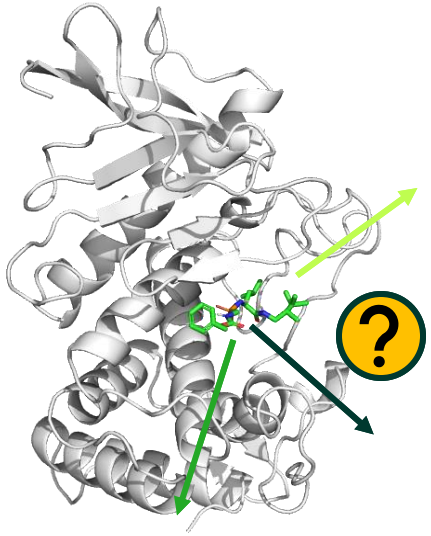
Import protein–ligand complex

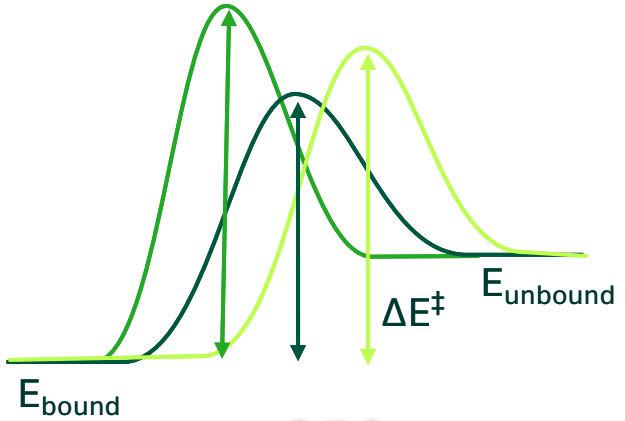
Identify Unbinding Trajectories

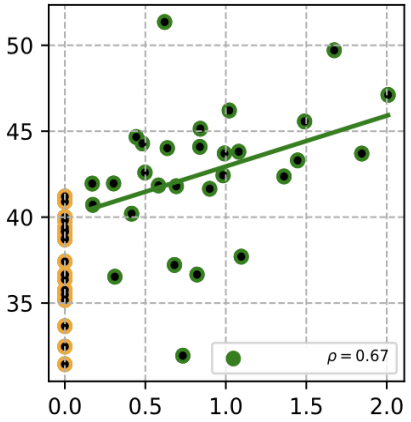
Calculate Energy along Trajectories

Extract Lowest Transition State Energy









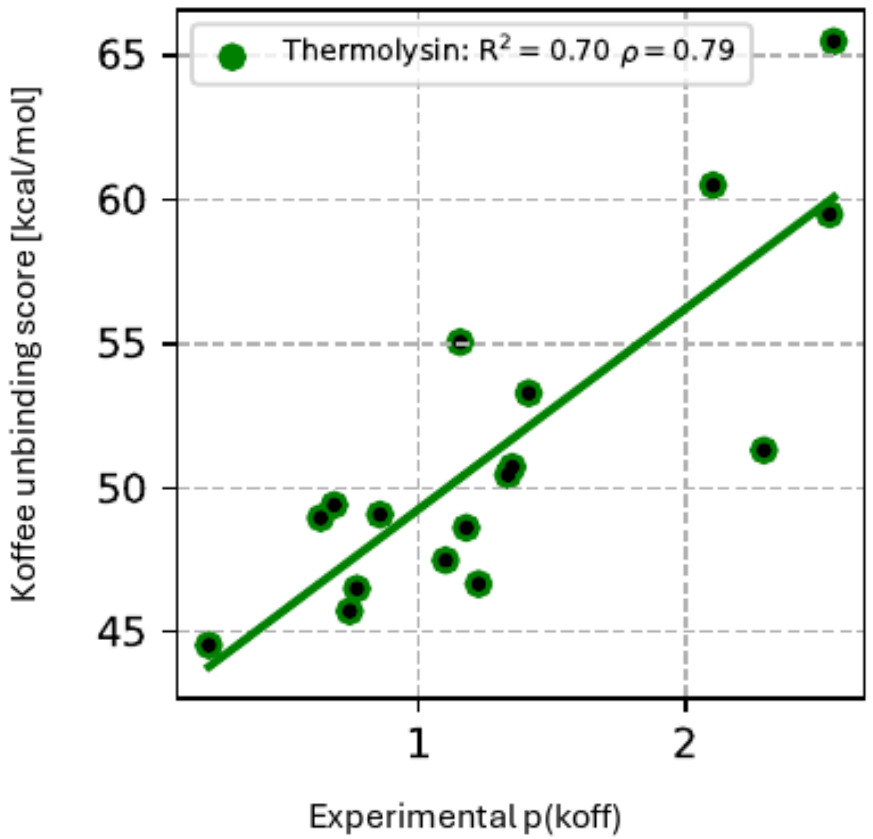
~1 GPU minute per complex*

AIDDD 2026

* EC2 g4dn.xlarge instance (NVIDIA T4 GPU, 4 vCPUs, 16 GB RAM), median runtime across 402 protein-ligand complexes was 96 seconds

kvantify

Force-field simulations can rank Thermolysin residence times.



Thermolysin: 17-ligand benchmark

- Classical force-field (FF) calculation
- 1 GPU-minute per ligand
- Rank correlation: 0.79

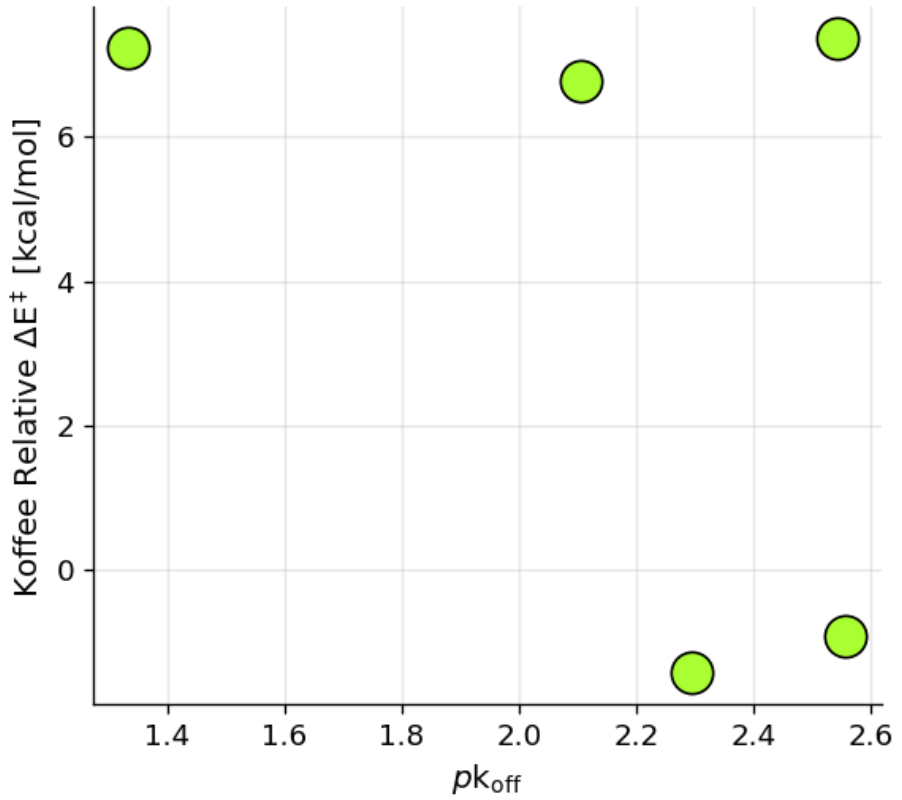
Fast and useful classical predictions.

So, what is the probem?

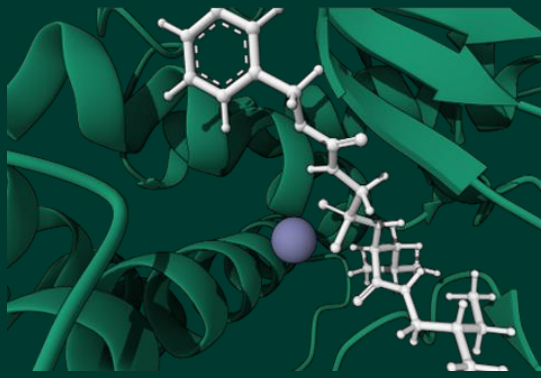
Madsen, Ziolek et al. | JCIM 66(17), 11377 | Thermolysin benchmark, Fig. 2a.

kvantify

Zooming into a specific subset of the ranked ligans reveals misrankings of the most potent ligands.



Separation by ligand charge close to a metal center



- One charge class (+1) ranks well.
- More potent class (+2) misranked.
- No indication in the screening results

Could electronic-structure (ES) calculations help?

AIDDD 2026

From isolated calculations to routine electronic structure calculations in drug discovery.

Current state

- Fast models guide decisions.
- Electronic-structure calculation adds ad-hoc detail for selected cases.

Problem

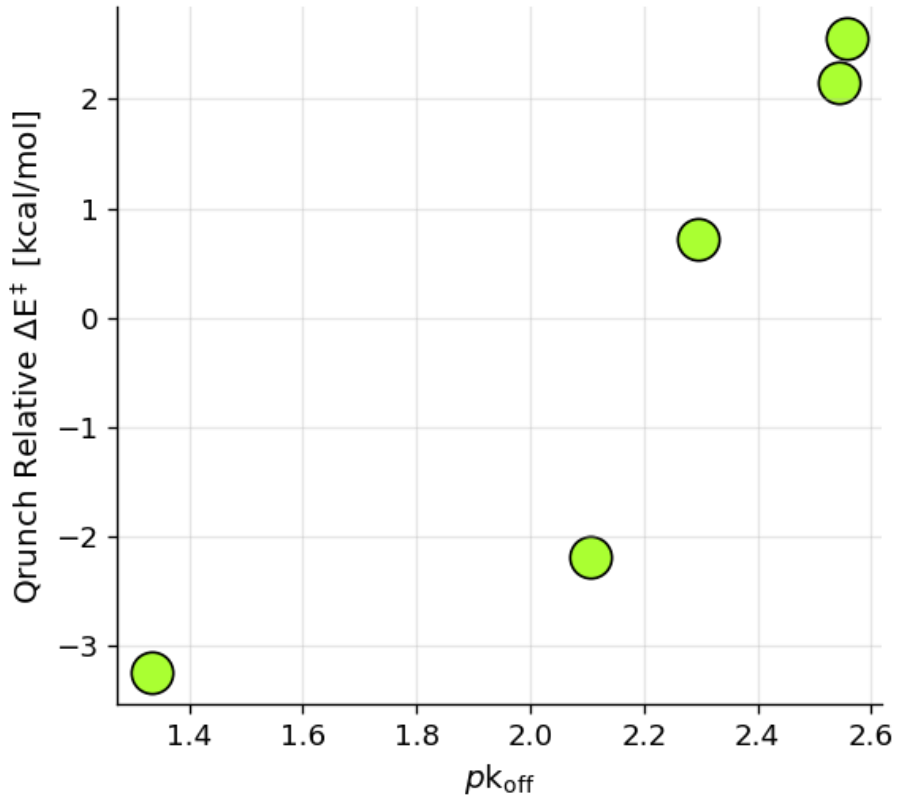
- Electronic structure calculations are slow
- Fast models often do not provide hints about misrankings
- Where and how to look more closely?

Question

How can we make quantum chemistry a routine, useful part of drug discovery?

Routine means accessible, repeatable and useful where justified, not calculation on every compound.

Today's (classical) electronic-structure methods recover the improved ligand ranking for Thermolysin ...



Same five Thermolysin ligands

- Start from Koffee's kinetic information.
- Align the structures. Tricky bit!
- Run (classical) electronic-structure calculations.

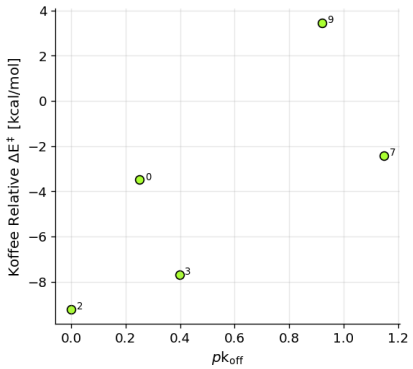
AIDDD 2026

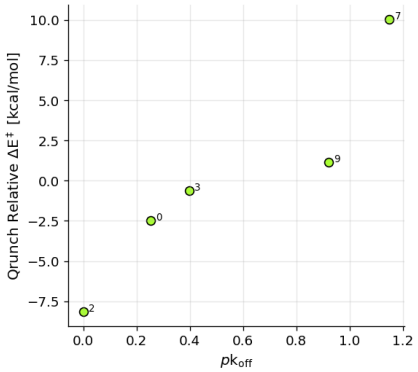
… and for other ligand-protein complexes, with pocket-dependent limits.

FF-energy

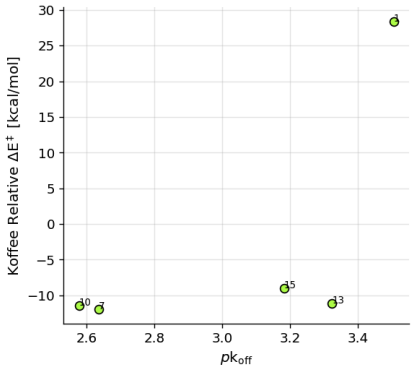
ES-energy

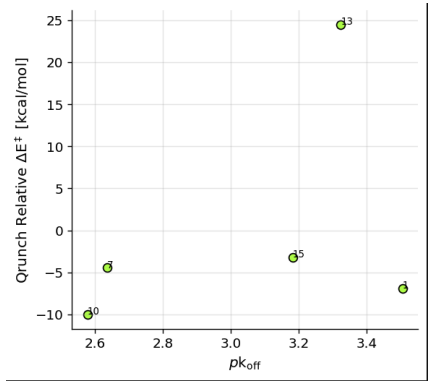
Works: FAK





Harder: sEH





What we learn

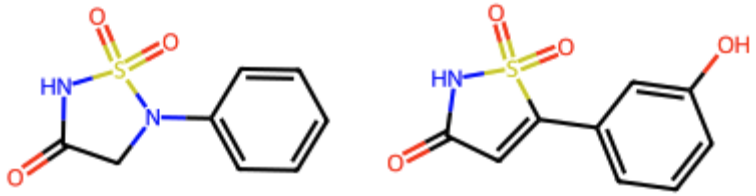
- The electronic-structure treatment matters.
- Pocket and interactions set the model's limits.
- **Expert setup** is still needed.

Next: Test and relax the model assumptions.

AIDDD 2026

The technology is transferable to activity-cliff investigations and other ligand-protein interactions.

PTP1B: 2CM8 is more potent



1. Take Koffee's two states.
2. Prepare a local model.
3. Compare methods.

Method	2BGE	2CM8
Experiment*	2.79	**5.86**
Global-FF**	**33.5**	30.7
Local g-xTB**	12.1	**17.2**
Local Qrunch**	13.5	**19.0**

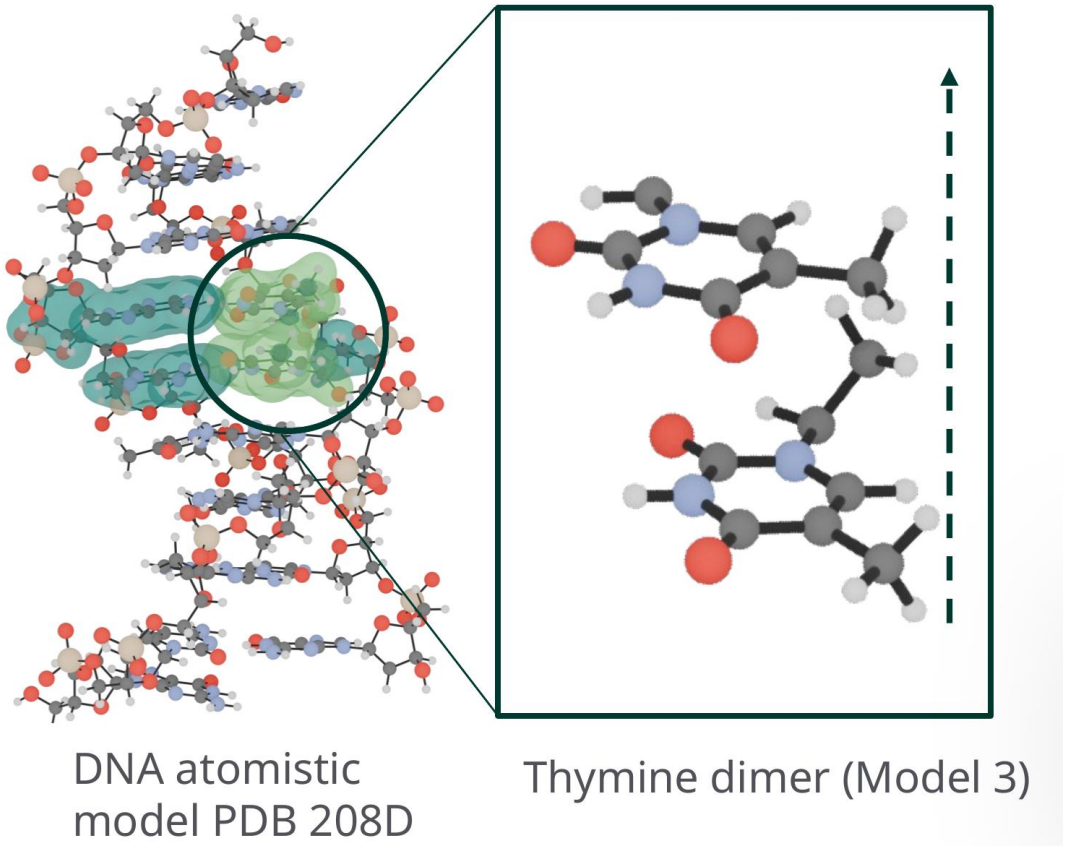
*Experimental potency

**Calculated energy difference [kcal/mol]

Electronic structure calculations improve output quality

AIDDD 2026

Electronic structure calculations are inevitable when dispersion effects are important.



DNA atomistic model PDB 208D

Thymine dimer (Model 3)

How can we test dispersion with electronic structure/quantum algorithms?

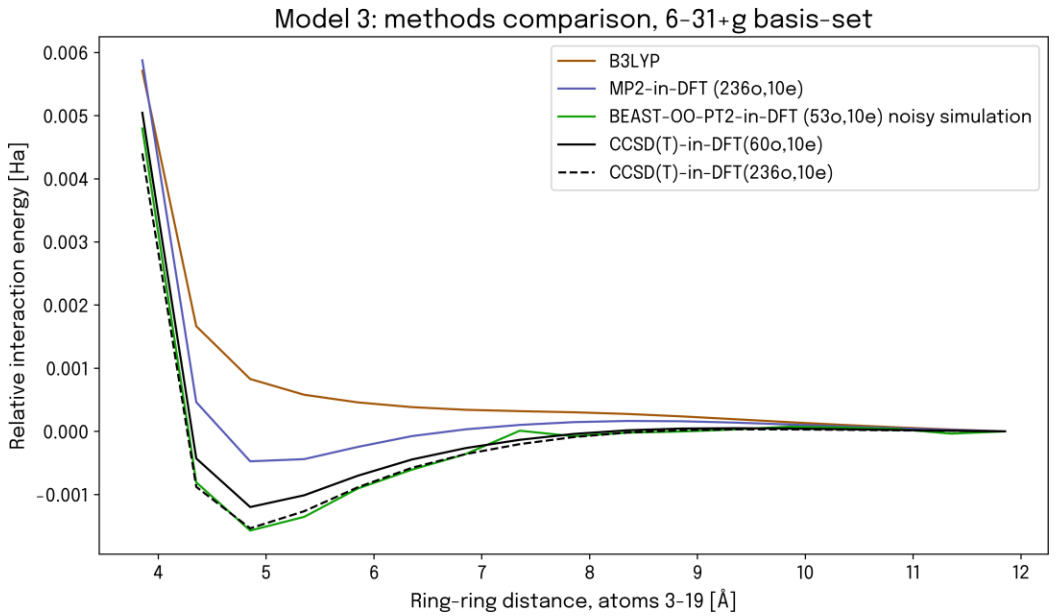
- Dispersion contributes to molecular recognition.
- Scan the distance between the rings.
- Compare the interaction energy with classical references.

AIDDD 2026

Kvantify Q2B, September 2026 | Thymine dimer, DNA-inspired model | Not a binding-affinity prediction.

kvantify

A smaller OO-BEAST-PT2 treatment tracks the larger CCSD(T) reference in this scan.

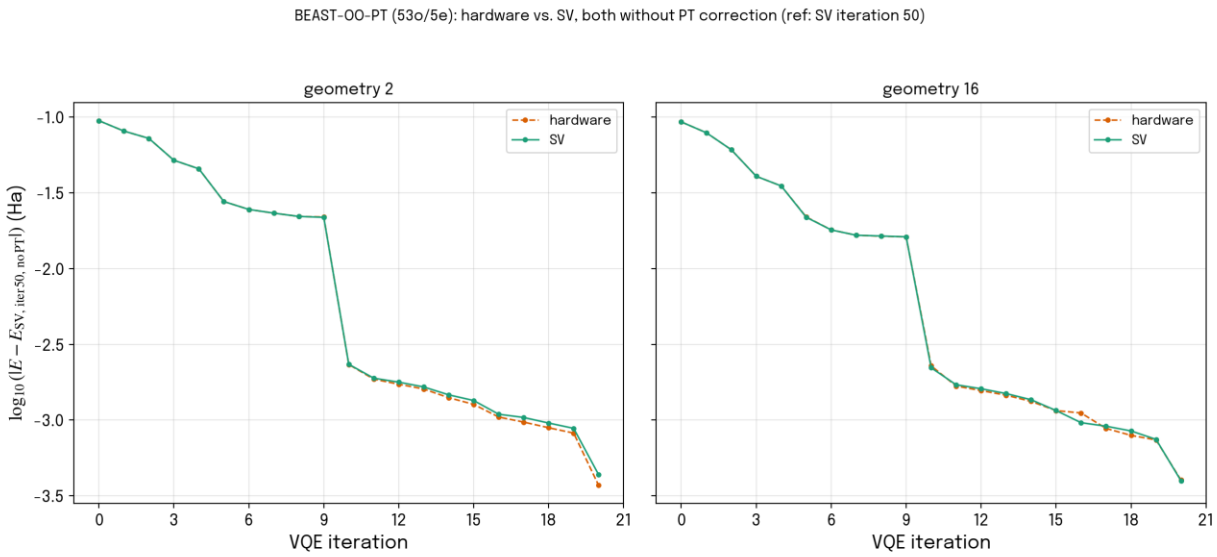


Comparing classical reference calculations:

- DFT does not include dispersion at all
- MP2 does, but not good enough
- CCSD(T) is the classical gold-standard
- **OO-BEAST-PT2 @ 52 orbitals matches CCSD(T) @ 236 orbitals**
- No claim of quantum advantage

AIDDD 2026

Quantinuum hardware closely follows the simulator at two selected geometries, establishing hardware viability.



- Quantinuum quantum hardware
- Exact state-vector simulator on NVIDIA GPUs
- Agreement is not advantage.

AIDDD 2026

Kvantify Q2B, September 2026 | Geometries 2 and 16 | Without PT correction | Quantinuum results review pending.

This shows that we can obtain useful accuracy on selected cases. Next is to work towards competitive end-to-end effort.

What the examples establish

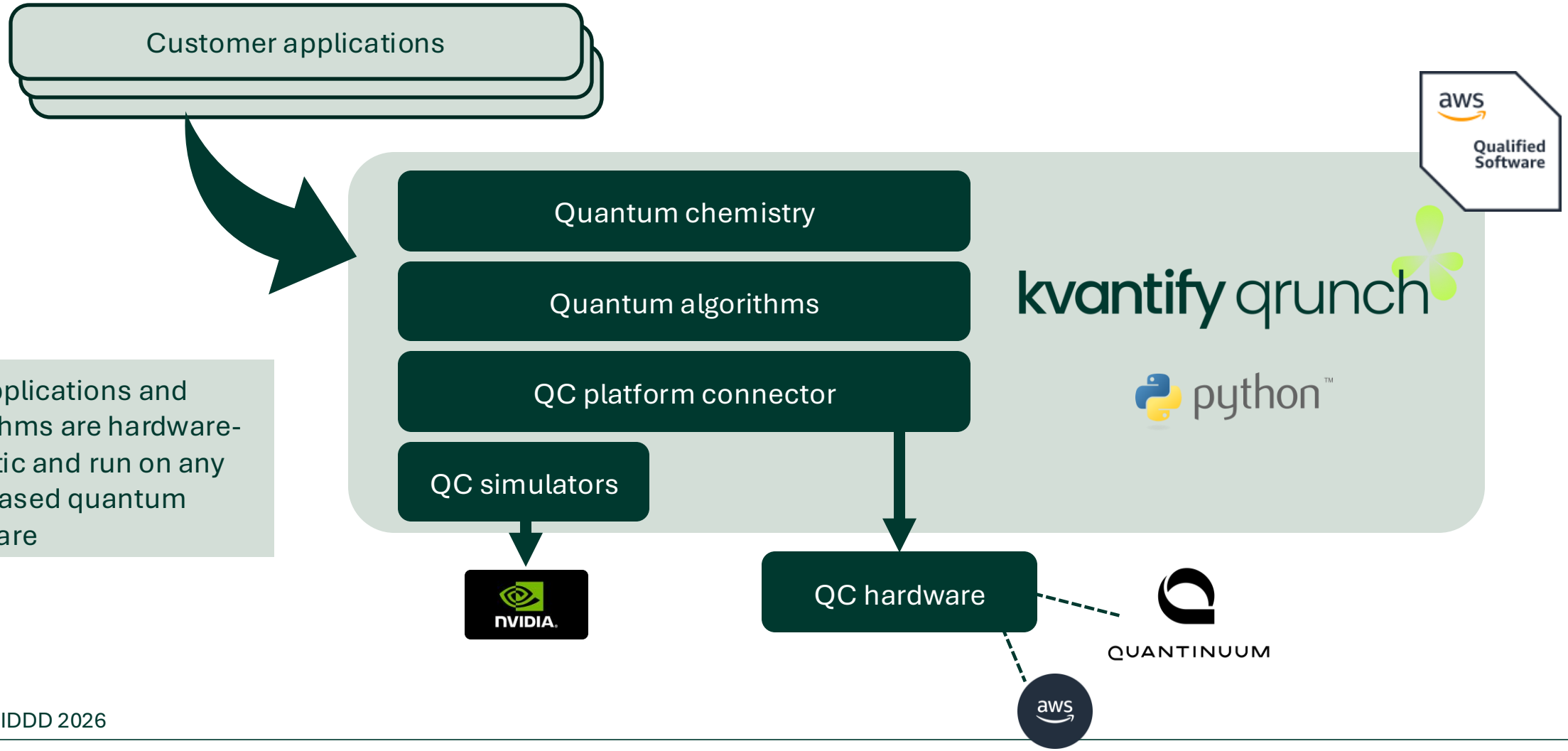
- Local (electronic structure) models can improve a ranking.
- We can describe intricate quantum effects with quantum heuristics today.
- The hardware is ready.

What is missing?

- Generalization of the algorithms for more complicated pockets.
- Streamlined implementations.
- Data for testing / More examples

Next: build an end-to-end pipeline with useful accuracy at competitive cost.

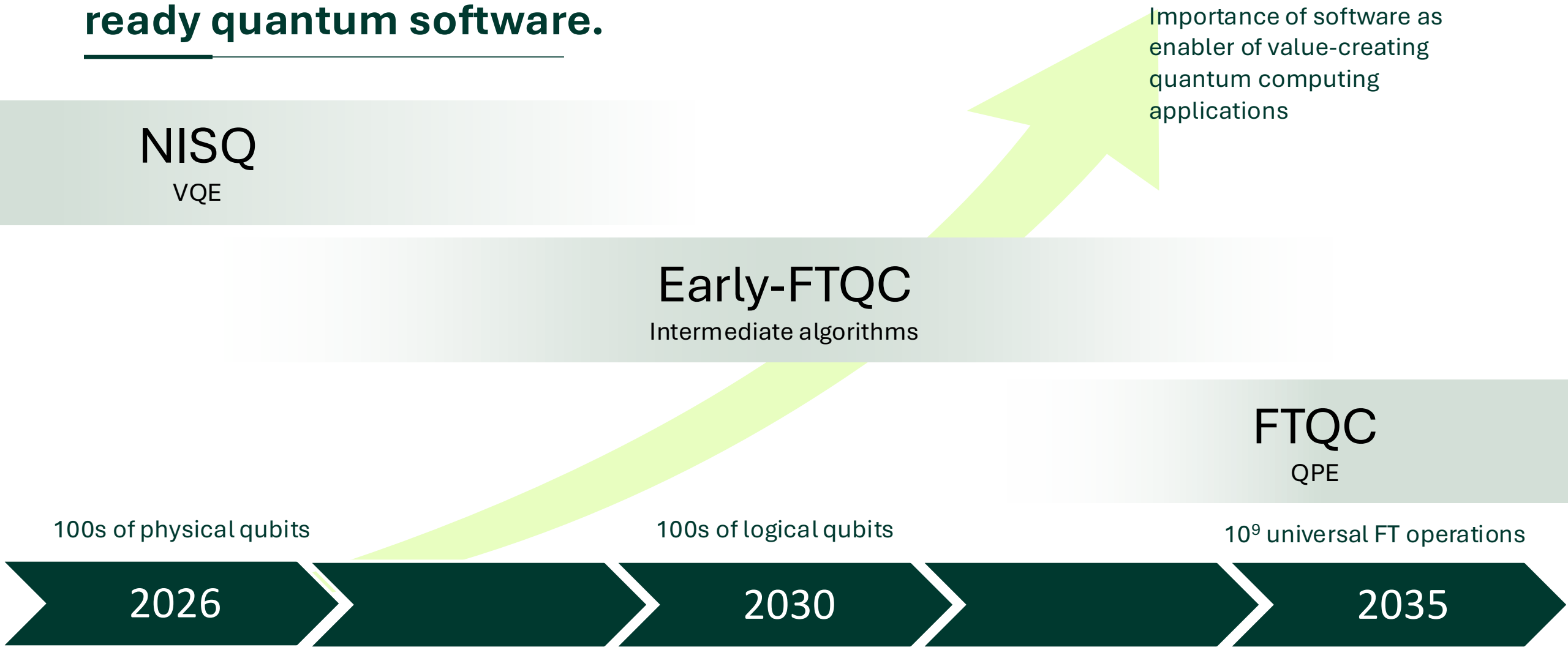
Kvantify Qrunch makes it easy for computational chemists to run calculations on any quantum computer.



Our applications and algorithms are hardware-agnostic and run on any gate-based quantum hardware

Source: Kvantify Q2B presentation, September 2026, slide 4 | Official Qrunch overview.

Qrunch tracks the moving hardware target by delivering industry-ready quantum software.



kvantify

Which unresolved decision in your history or pipeline could we investigate this way?

Your problem

- Unexpected ranking, activity cliff or unexplained interaction?
- Structures, measurements and a current prediction?
- A result that could change your next decision?

A joint investigation

- Identify the physical explanation to test.
- Build a model and compare with credible baselines.
- Assess accuracy, effort, cost and decision value.

Selected examples demonstrate the approach; usefulness for your case is what we would test together.

kvantify

THANK YOU

Transforming molecular discovery by coupling quantum and classical computing