
AWS
re:Invent
NOV. 28 – DEC. 2, 2022 | LAS VEGAS, NV

PRT278

SPONSORED BY INTEL

How Intel & AWS collaborate to solve some of the world's most urgent issues

Akanksha Bilani (she/her)
Go to Market Lead,
AWS Account Team
Intel

Tanner Marsh (he/him)
Associate
Dana Farber/Harvard Cancer Center

Arman Zaribafiyan
Founder and CEO
Good Chemistry Co

M. Nicolas Do Huu
Chief Technology Officer
IKTOS

© 2022, Amazon Web Services, Inc. or its affiliates. All rights reserved.

Leveraging the power of HPC: Impactful computing

Akanksha Bilani (she/her)

Go to Market Lead, AWS Account Team
Intel

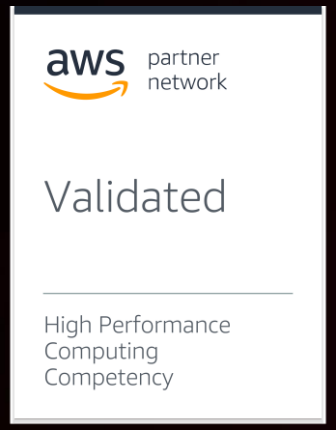
© 2022, Amazon Web Services, Inc. or its affiliates. All rights reserved.

Committed to driving HPC innovation

"Intel is a very deep partner of AWS and will be for a long time. That's not changing."

Andy Jassy, President and CEO, Amazon







© 2022, Amazon Web Services, Inc. or its affiliates. All rights reserved.

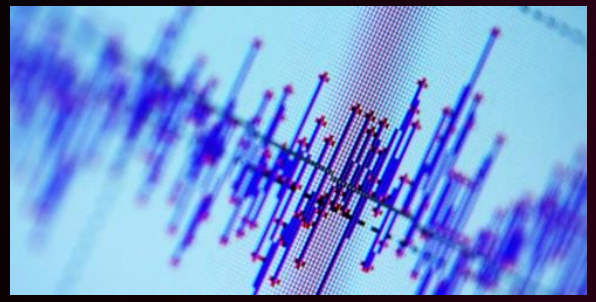
HPC for social impact



Life sciences



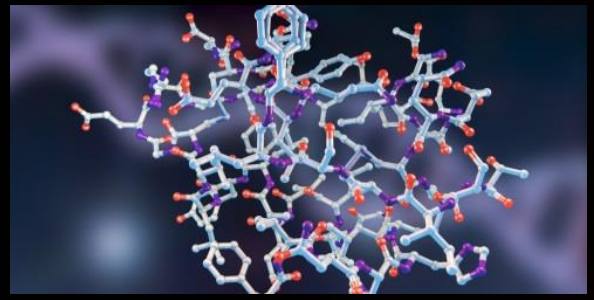
Financial – Risk



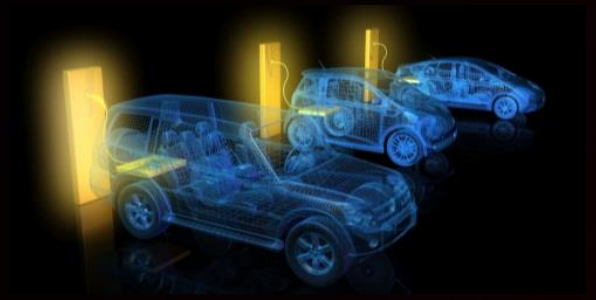
Energy



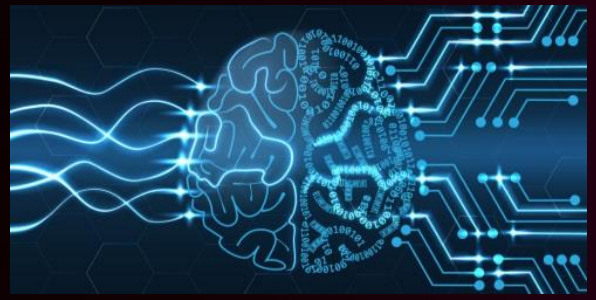
Weather



Scientific visualization/
professional rendering



Simulation,
CAE & CFD



Data analytics &
machine learning

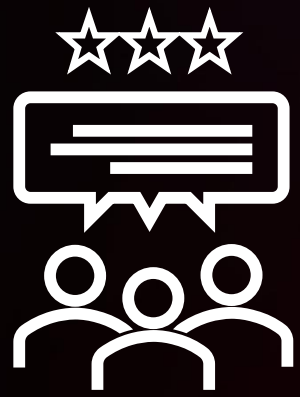


Defense/security

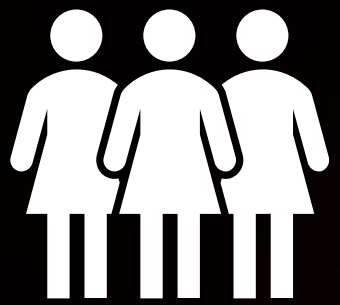
aws

© 2022, Amazon Web Services, Inc. or its affiliates. All rights reserved.

Intel & AWS share a joint commitment to:



Putting customers first



Improving lives
with technology



Shaping the future
of technology

© 2022, Amazon Web Services, Inc. or its affiliates. All rights reserved.



Democratizing cancer research with the largest known HPC run

Tanner Marsh (he/him)
Associate
Dana Farber/Harvard Cancer Center

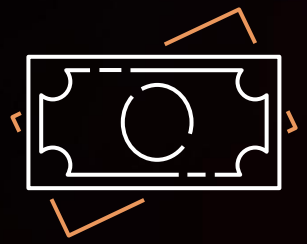
aws
© 2022, Amazon Web Services, Inc. or its affiliates. All rights reserved.

Innovating drug discovery



~40

New drugs approved annually



$2–3B

average costs per drug



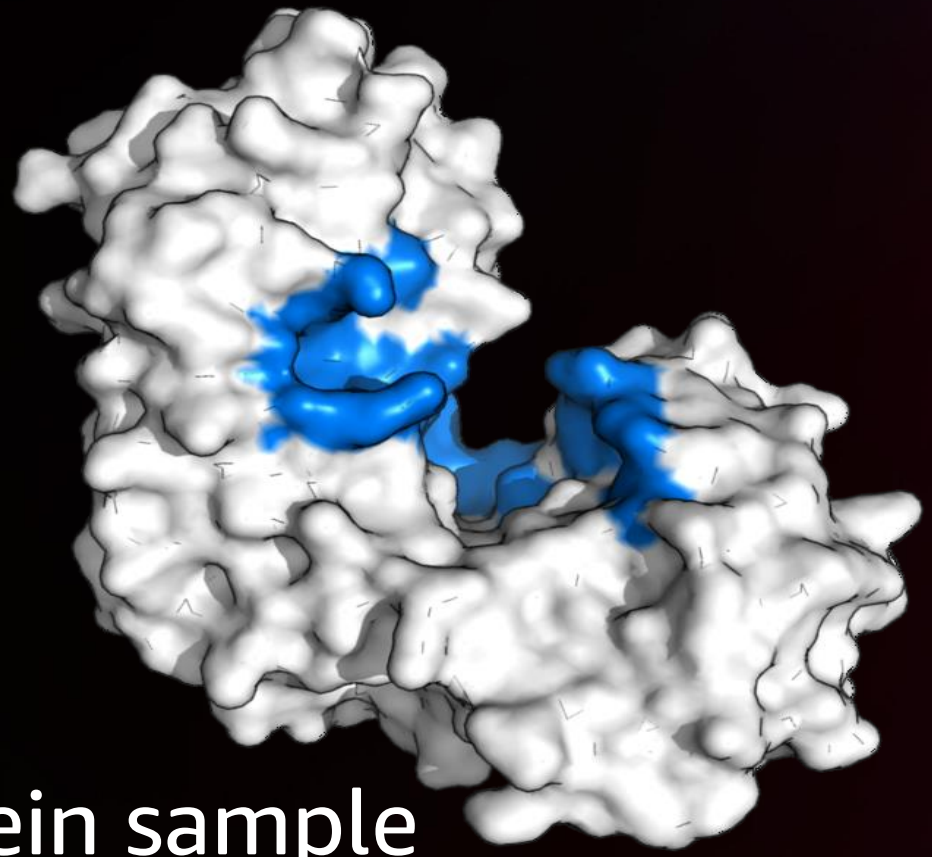
10–12 years

average drug development and approval time

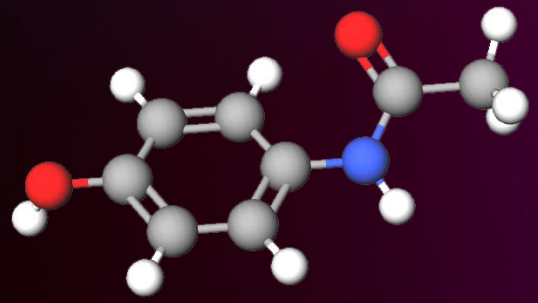
aws

© 2022, Amazon Web Services, Inc. or its affiliates. All rights reserved.

Treating “untreatable” cancers



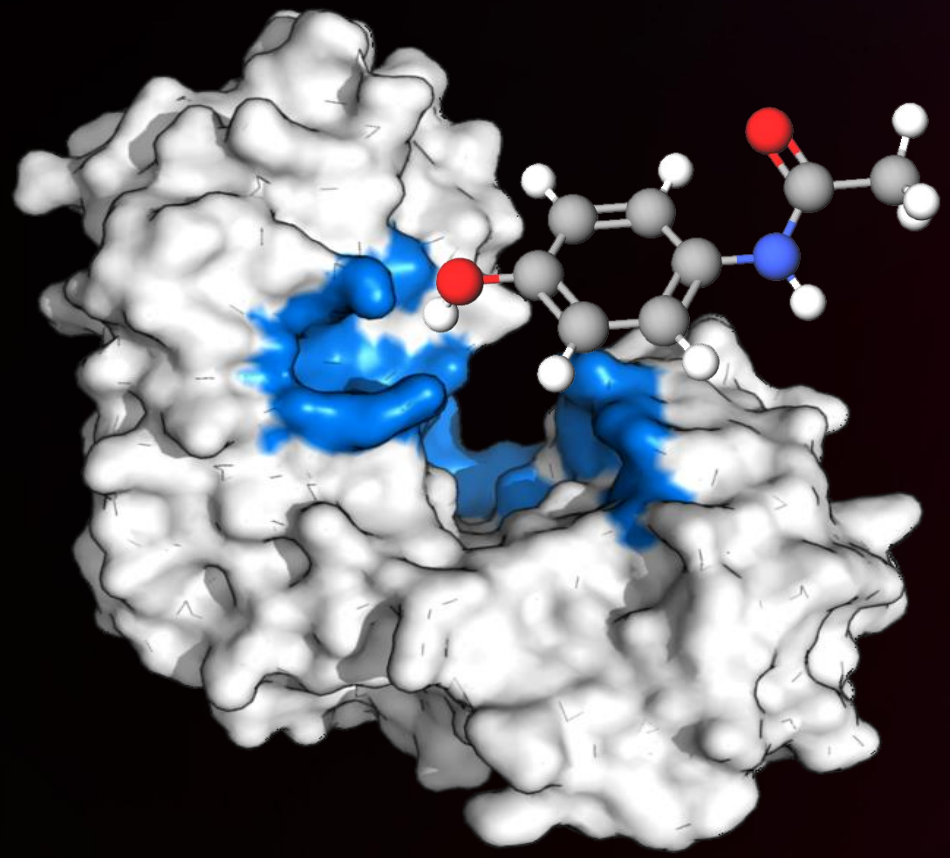
Protein sample



Drug candidate

© 2022, Amazon Web Services, Inc. or its affiliates. All rights reserved.

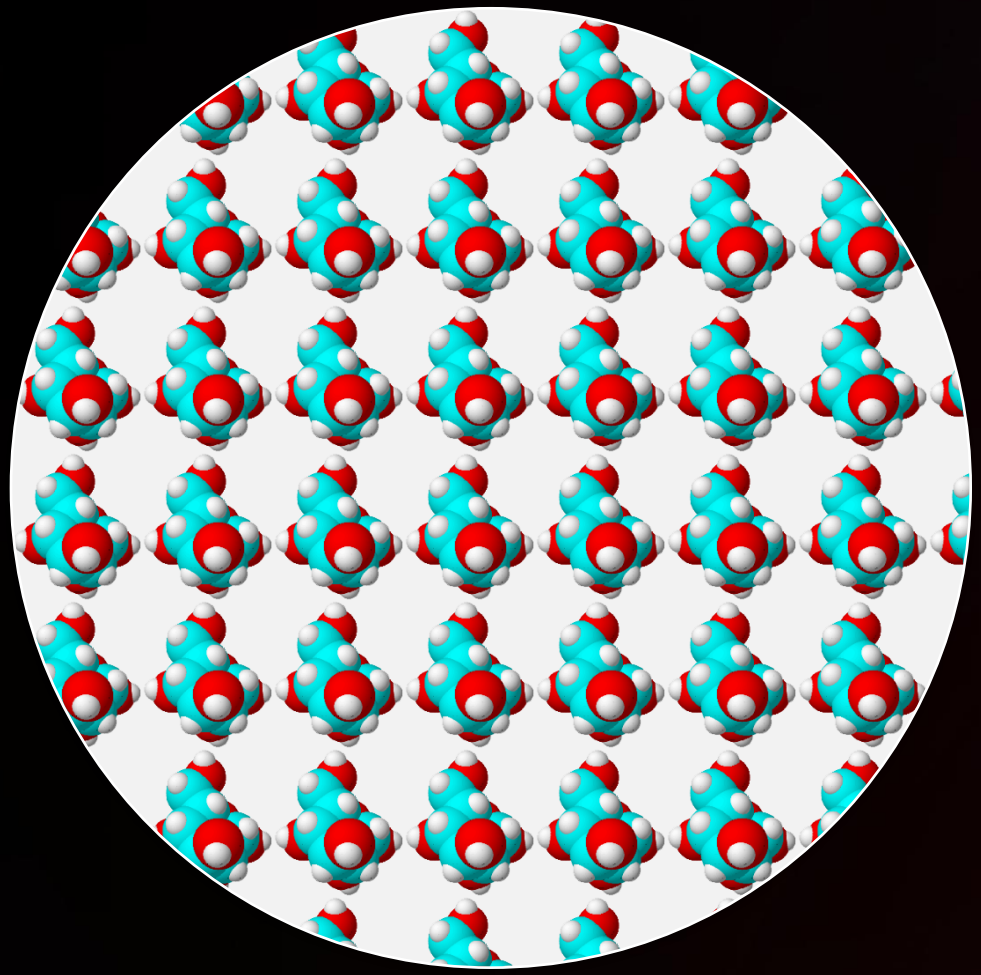
Treating “untreatable” cancers



Does it fit?

© 2022, Amazon Web Services, Inc. or its affiliates. All rights reserved.

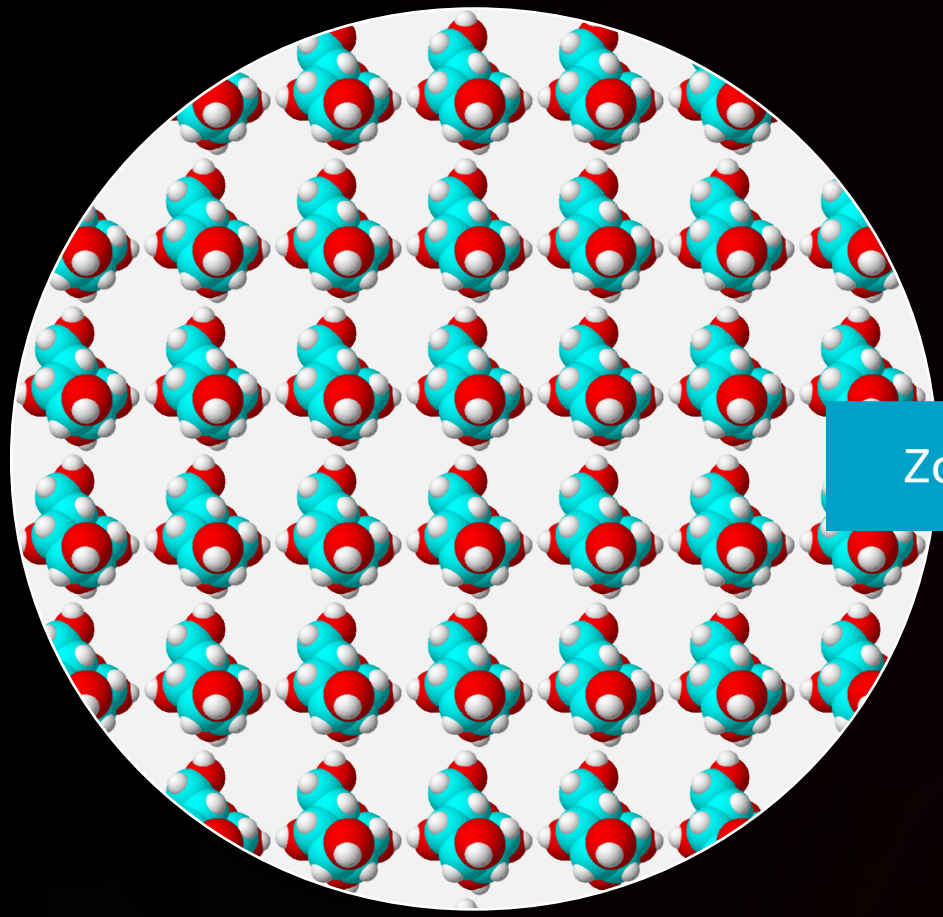
Leveraging hyperscale compute



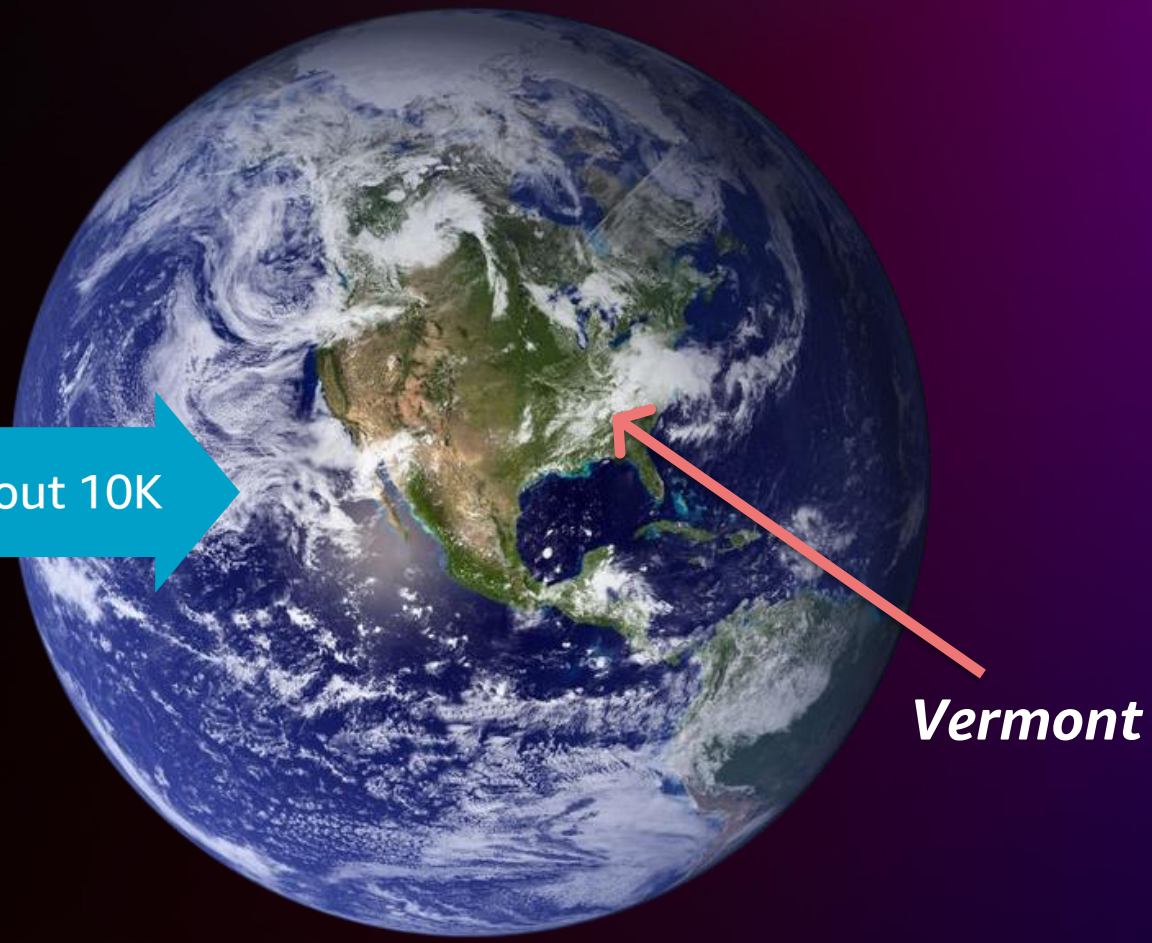
100K–1M molecules
(traditional screening library)

© 2022, Amazon Web Services, Inc. or its affiliates. All rights reserved.

Leveraging hyperscale compute



Zoom out 10K



100K molecules
(traditional screening library)

100K molecules – In a
1B virtual chemical space

aws
© 2022, Amazon Web Services, Inc. or its affiliates. All rights reserved.

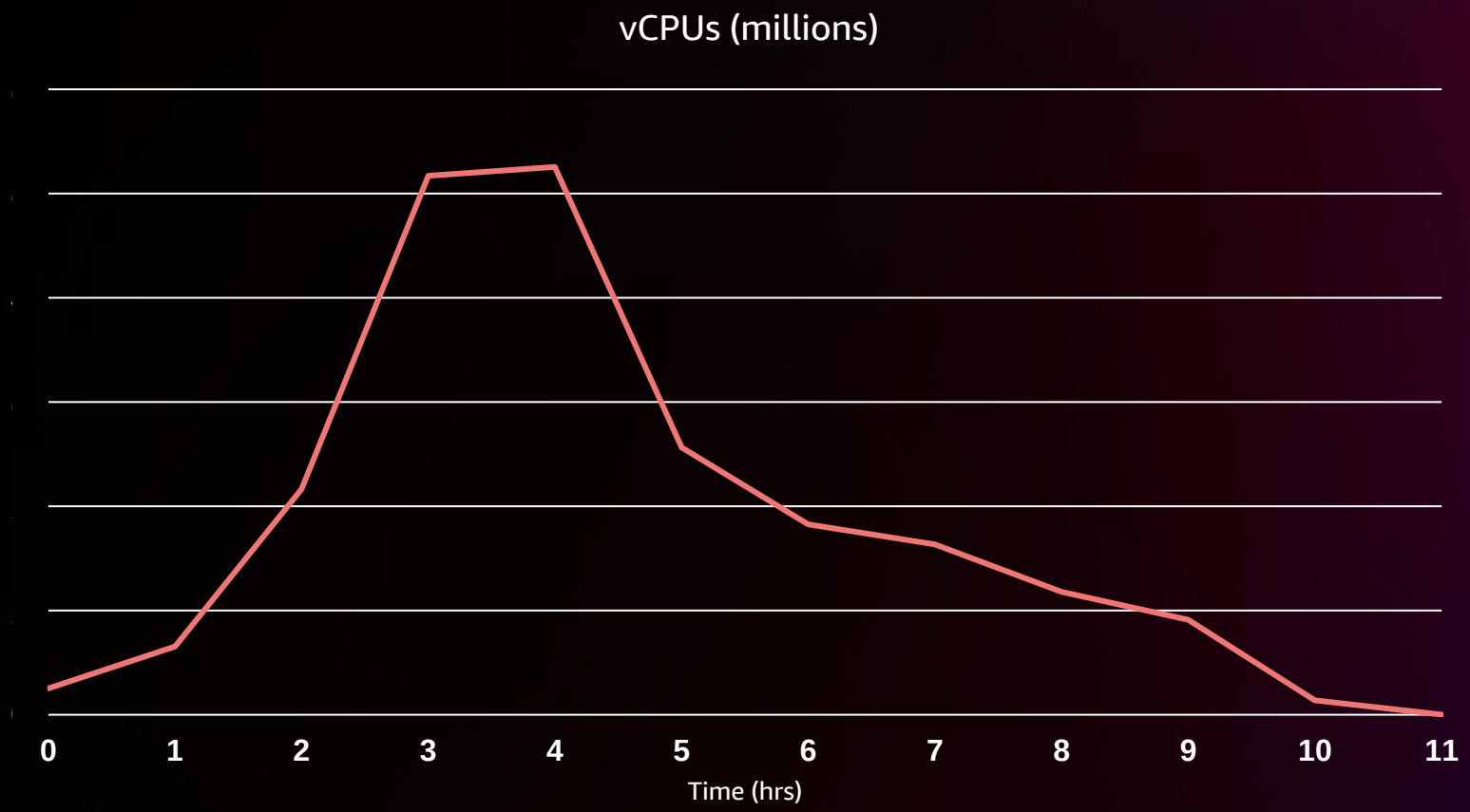
Democratizing drug discovery



aws

© 2022, Amazon Web Services, Inc. or its affiliates. All rights reserved.

Learning from largest known HPC run in the cloud



5.7M vCPUs in <11 hours

aws
© 2022, Amazon Web Services, Inc. or its affiliates. All rights reserved.

GOOD CHEMISTRY
COMPANY

A chemistry supercomputer on the cloud to eliminate forever chemicals

Arman Zaribafiyan
Founder and CEO
Good Chemistry Co

aws
© 2022, Amazon Web Services, Inc. or its affiliates. All rights reserved.

Reimagining computational chemistry

10^{82}

atoms in the observable universe

10^{180}

possible molecules









© 2022, Amazon Web Services, Inc. or its affiliates. All rights reserved.

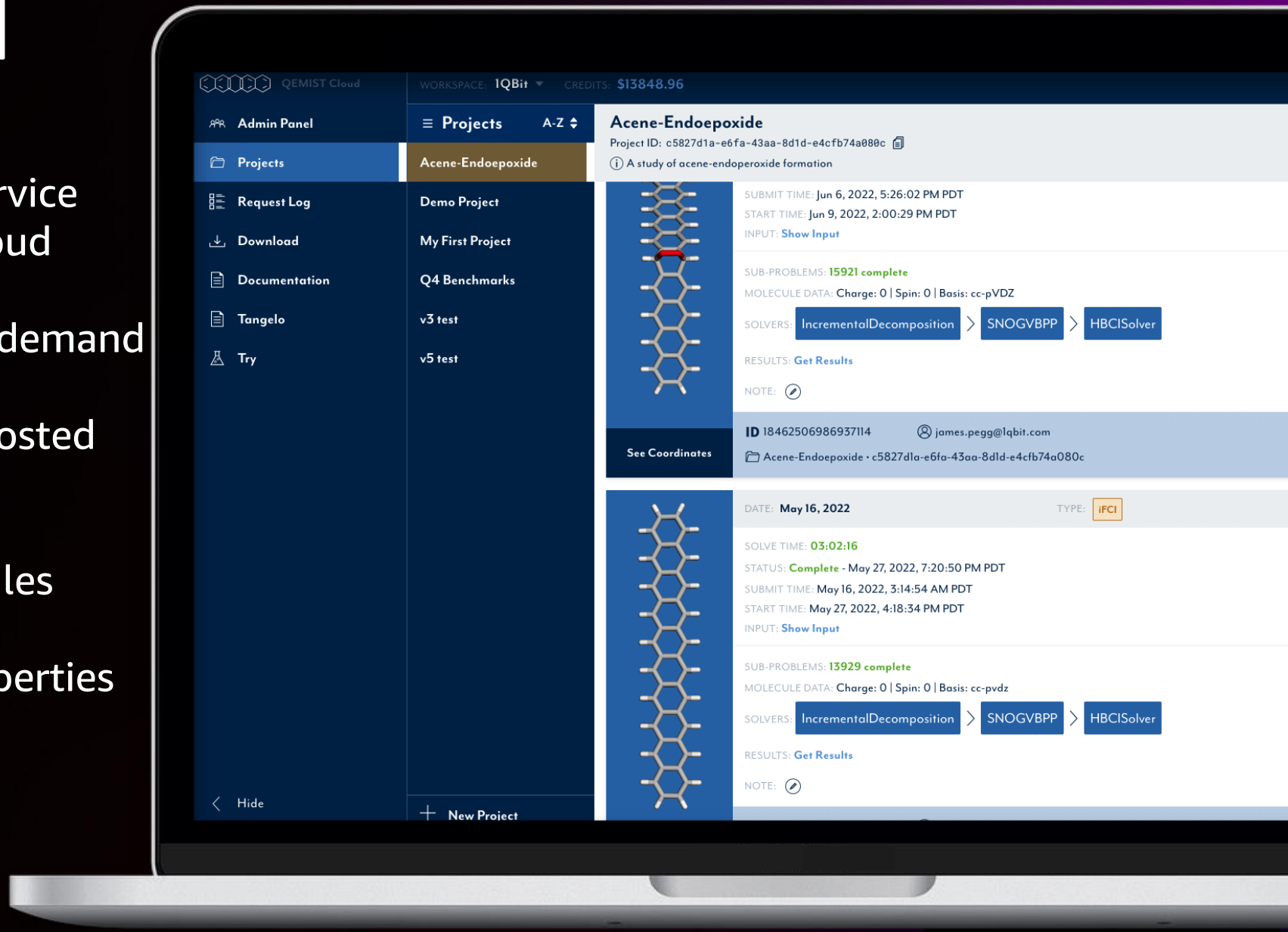
QEMIST Cloud

High-accuracy chemistry as a service
zero-CAPEX virtual lab in the cloud

Massively scalable compute, on demand

Cloud-optimized algorithms, boosted by AI, ML, quantum computing

Input: Representation of molecules
Output: Rapid simulation and prediction of their chemical properties



© 2022, Amazon Web Services, Inc. or its affiliates. All rights reserved.

Per- and polyfluoroalkyl substances (PFAS)



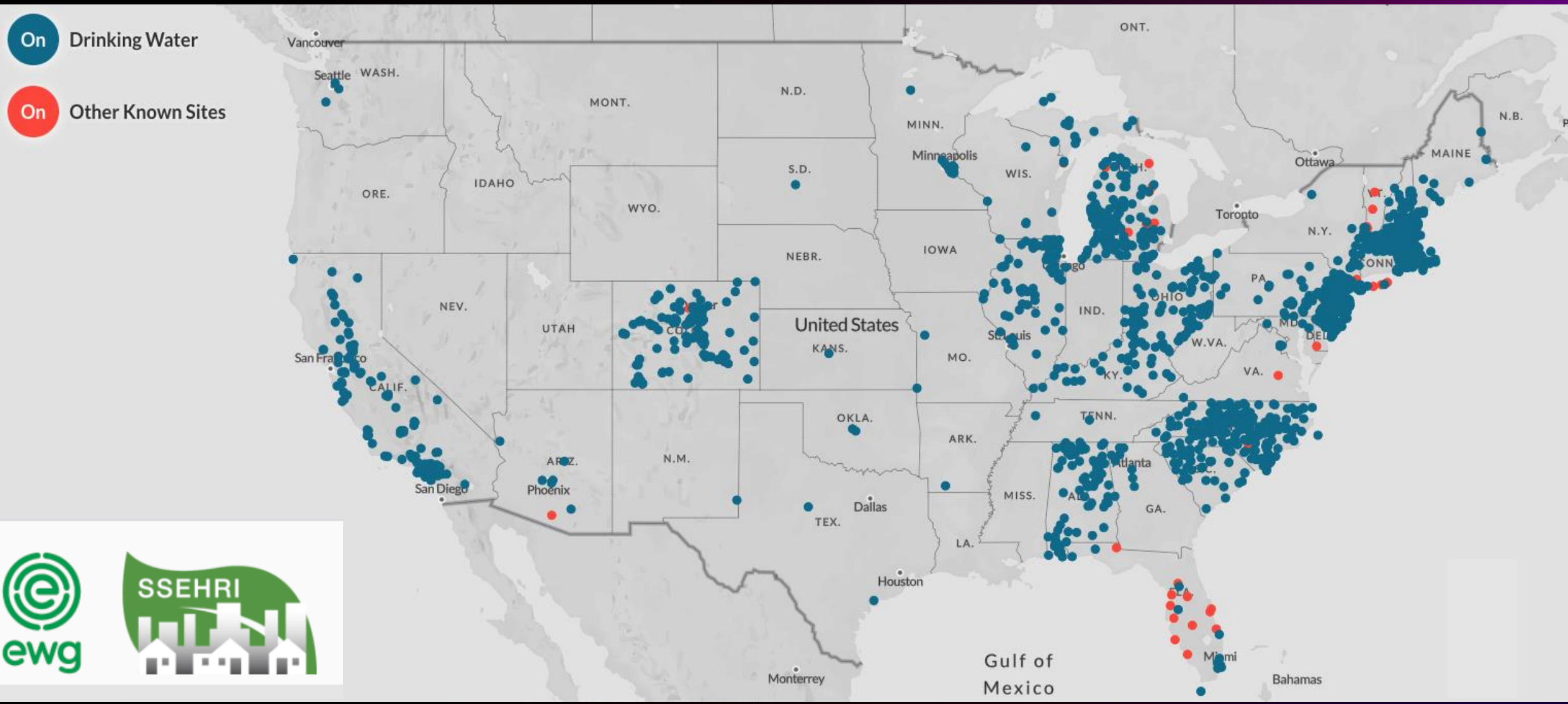






© 2022, Amazon Web Services, Inc. or its affiliates. All rights reserved.

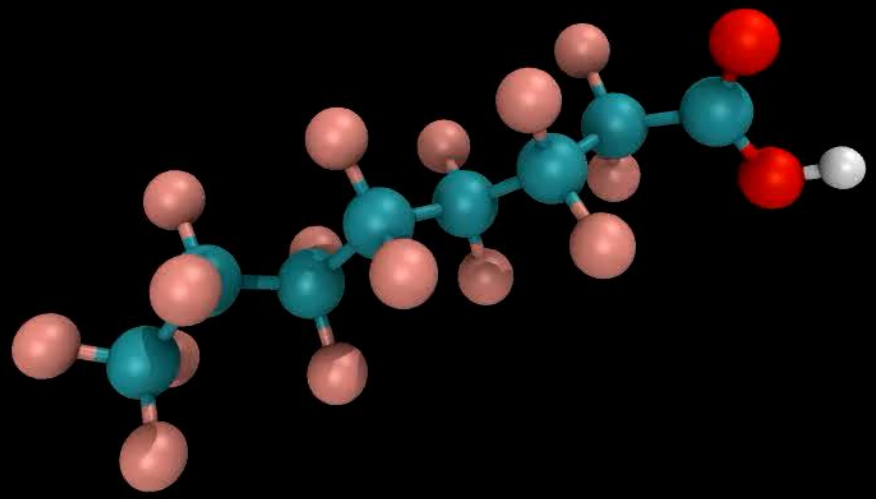
PFAS contamination in the US



© 2022, Amazon Web Services, Inc. or its affiliates. All rights reserved.

https://pfasproject.com/2020/04/23/mapping-the-pfas-contamination-crisis/

PFAS molecules: Prohibitively hard to break



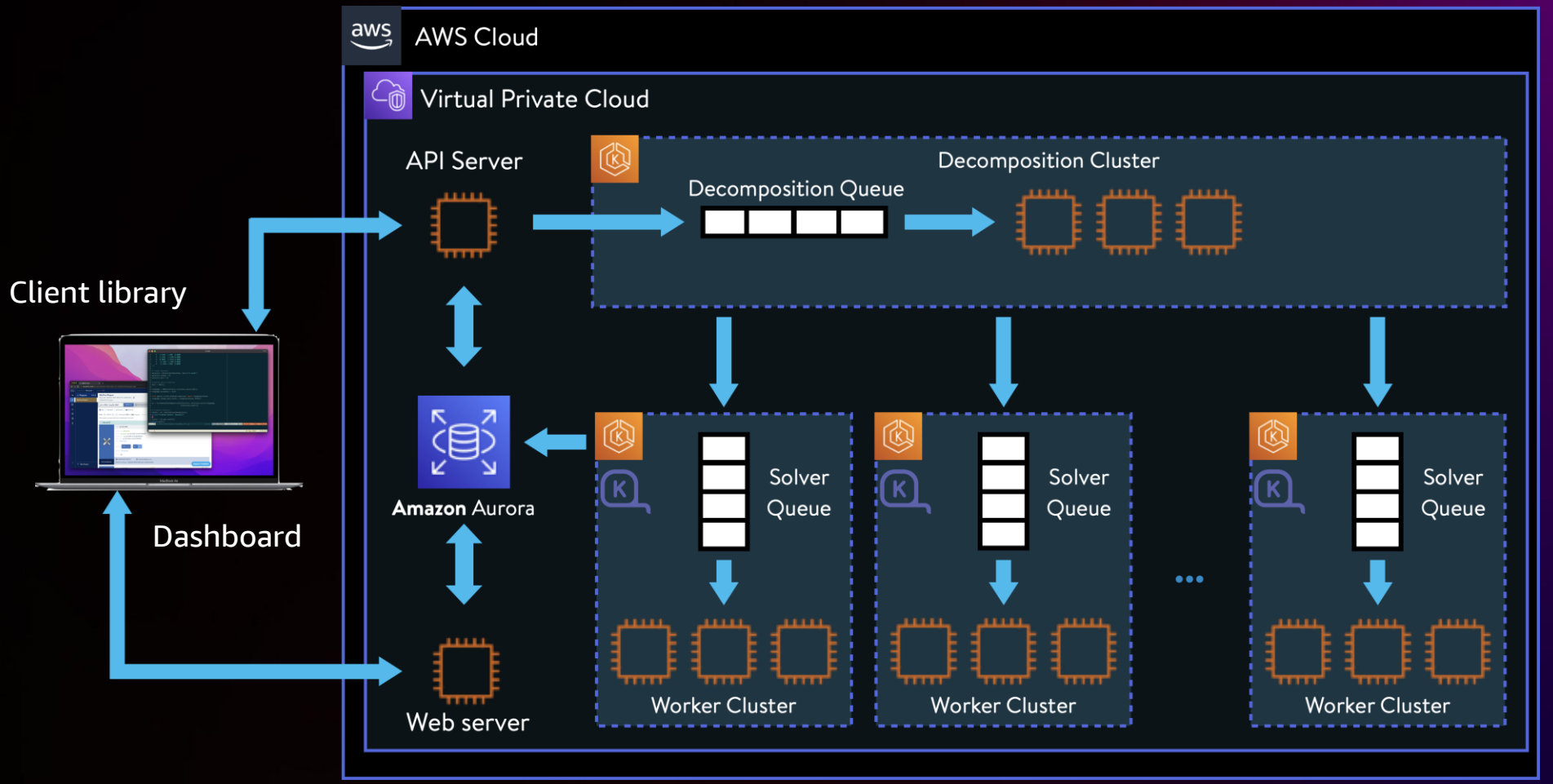
Exact solution requires the diagonalization of a 10^{151} x 10^{151} matrix

aws

© 2022, Amazon Web Services, Inc. or its affiliates. All rights reserved.

Supercomputer for chemistry on the cloud

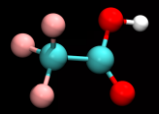
iFCI in QEMIST Cloud



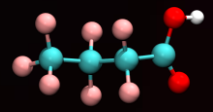
© 2022, Amazon Web Services, Inc. or its affiliates. All rights reserved.

Intractable made tractable

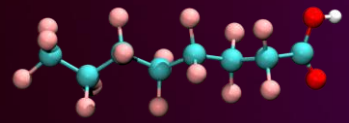
16K vCPUs ⟵ 1.1M vCPUs



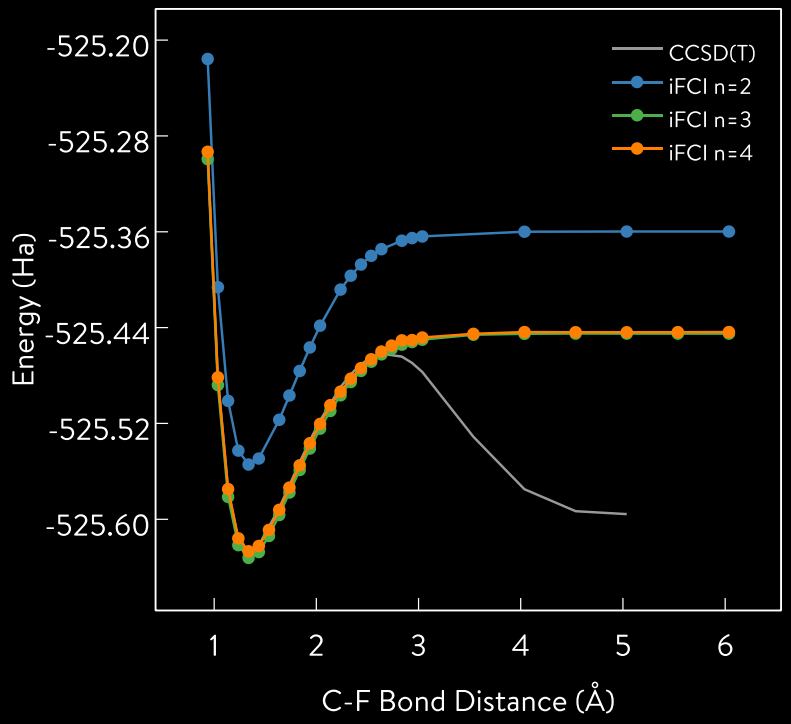
TFA: 10^{42}

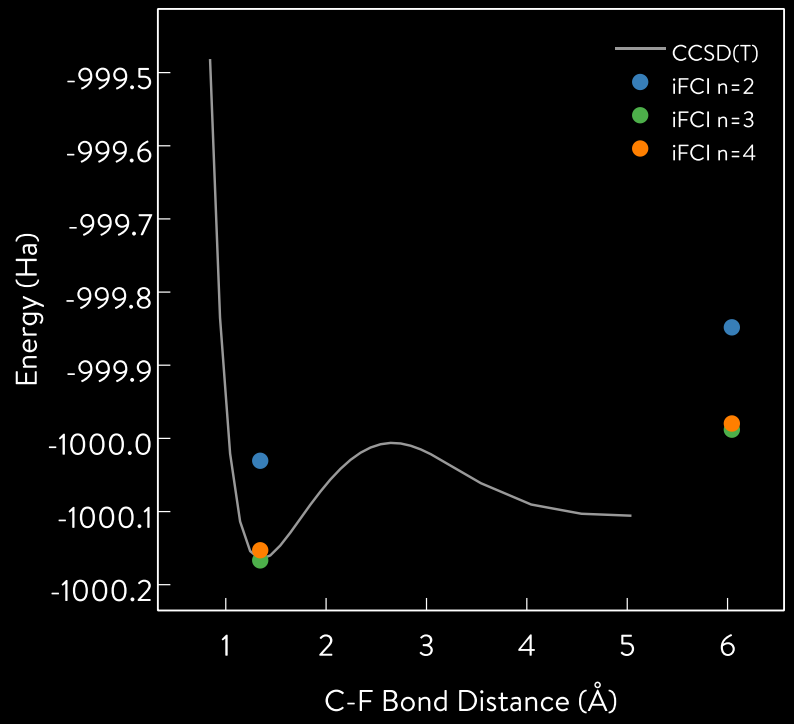


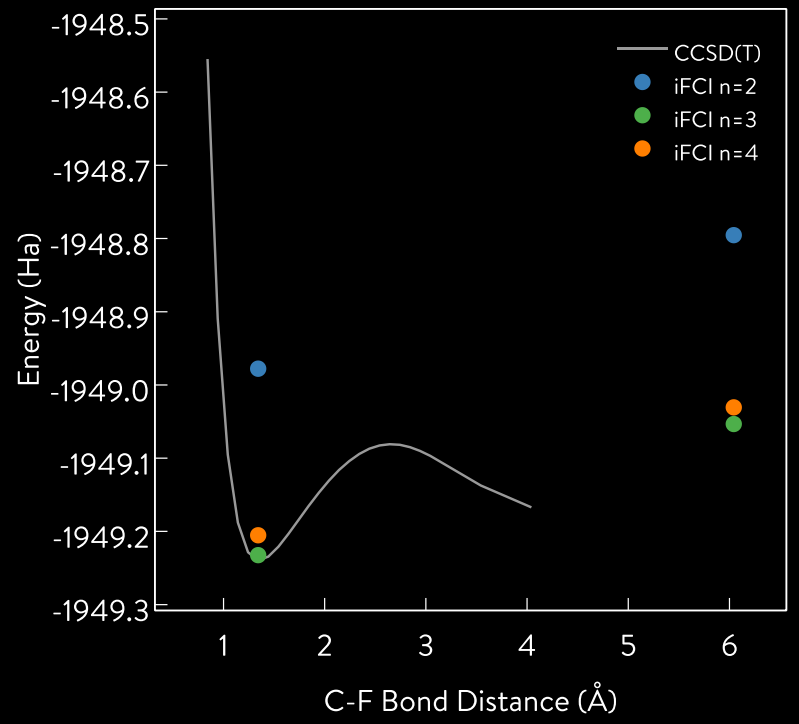
PFBA: 10^{78}



PFOA: 10^{151}







© 2022, Amazon Web Services, Inc. or its affiliates. All rights reserved.

Just the beginning









© 2022, Amazon Web Services, Inc. or its affiliates. All rights reserved.


GOOD CHEMISTRY
COMPANY
Get access to
QEMIST Cloud
today.
www.goodchemistry.com



Accelerating drug discovery for malaria

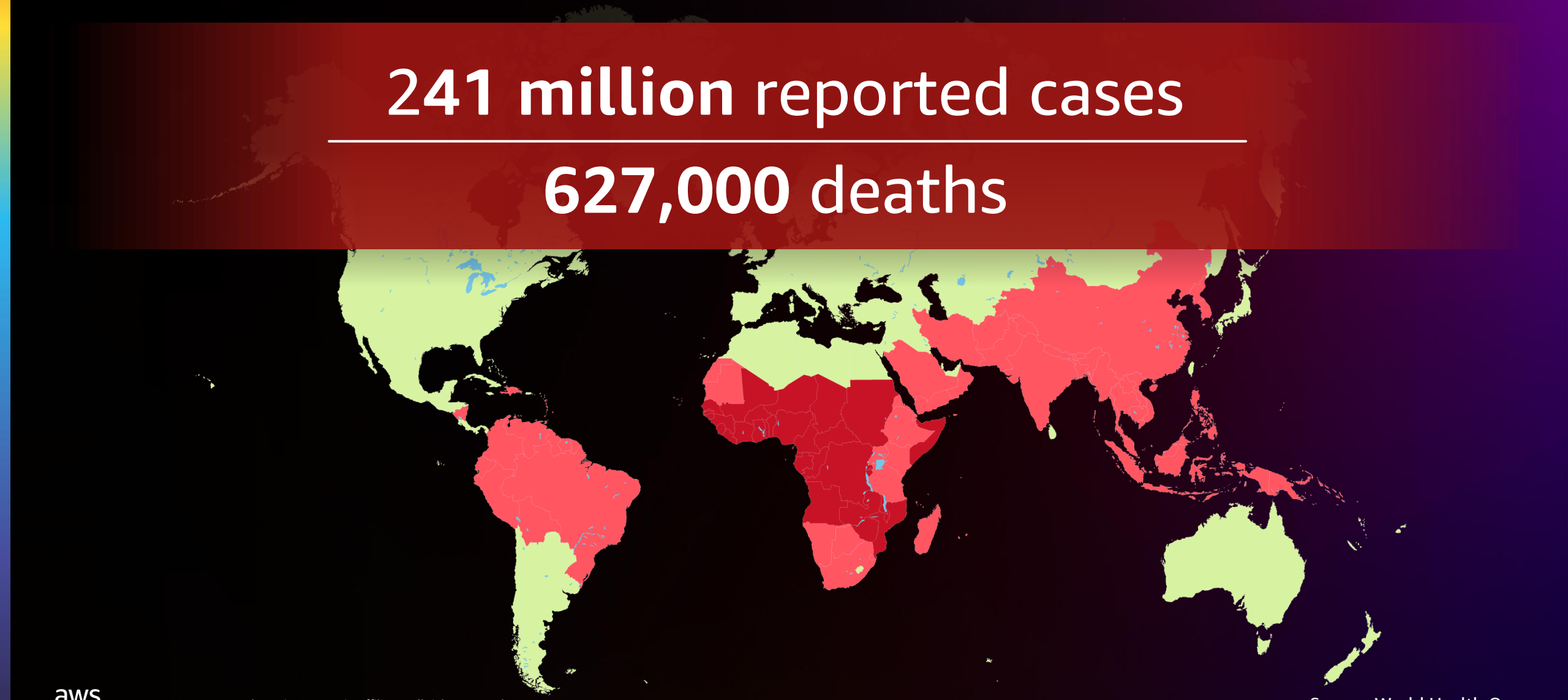
M. Nicolas Do Huu
Chief Technology Officer
IKTOS

© 2022, Amazon Web Services, Inc. or its affiliates. All rights reserved.

In 2020, malaria caused an estimated . . .

241 million reported cases

627,000 deaths



© 2022, Amazon Web Services, Inc. or its affiliates. All rights reserved.

Source: World Health Org

Iktos

AI technologies for medicinal chemistry to accelerate new drug discovery



Accelerating discovery, increasing success rate, and drastically reducing costs toward identification of a drug candidate

aws

© 2022, Amazon Web Services, Inc. or its affiliates. All rights reserved.

Medicines for Malaria Venture



MMV

Medicines for Malaria Venture

Discover, develop and deliver new, effective and affordable antimalarial drugs.

aws

© 2022, Amazon Web Services, Inc. or its affiliates. All rights reserved.

Source: https://www.mmv.org/

Need for a cost-effective virtual screening technology



Virtual screening is a computational approach of **hit discovery**

The goal is to find active compounds in a database of millions using **molecular docking simulations**

However, each simulation can run for **several minutes** which leads to a long and costly virtual screening campaign

aws

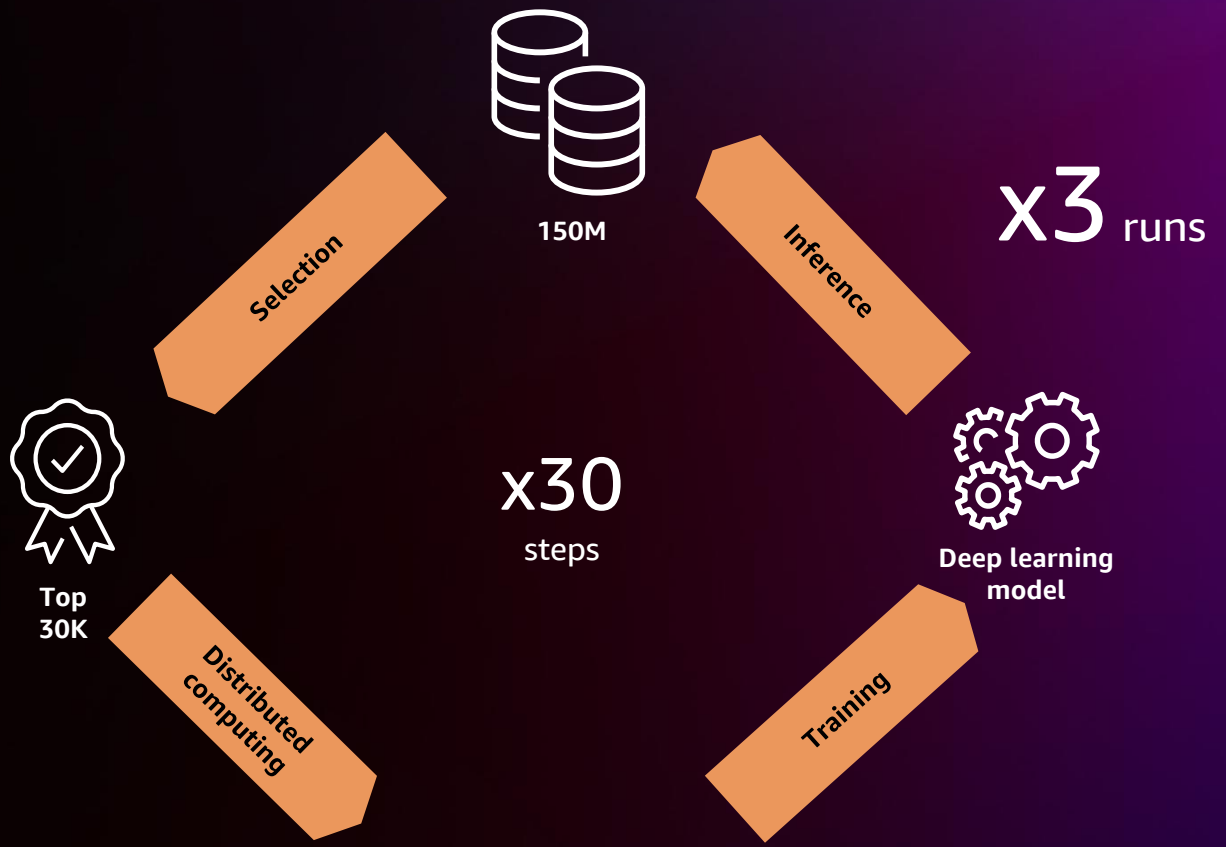
© 2022, Amazon Web Services, Inc. or its affiliates. All rights reserved.

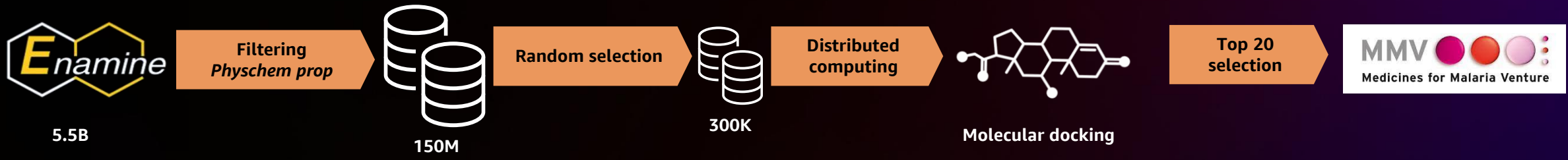
Dock AI: Accelerate virtual screening with active learning

© 2022, Amazon Web Services, Inc. or its affiliates. All rights reserved.

Dock AI for MMV

Finding hits by docking only
1% of the target database





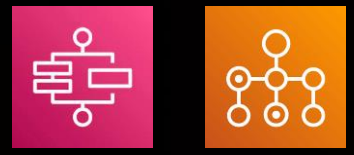
aws
© 2022, Amazon Web Services, Inc. or its affiliates. All rights reserved.

Technological components

© 2022, Amazon Web Services, Inc. or its affiliates. All rights reserved.

Technological components

Data preparation



AWS **Step Functions**

AWS **Batch**

- Simulations plus protonation software
- RDKit Python package for molecular descriptors and fingerprint calculation

HPU model training



- **Amazon EC2 DL1 instance**
- **Habana's Gaudi Accelerator**
- **PyTorch**

Distributed CPU inference



- Amazon EC2 C6i instances
- TorchServe
- **IPEX: Intel Extension for PyTorch**

Distributed docking

aws

AWS-CYCLONE-SOLUTION

High Performance HPC Scheduler for Massive Scale

- AWS Cyclone
- Dock6 docking software

aws

© 2022, Amazon Web Services, Inc. or its affiliates. All rights reserved.

Results

© 2022, Amazon Web Services, Inc. or its affiliates. All rights reserved.

Results (so far)

- 2 runs were performed
- 1.1M dockings per run : less than 1% of the database
- Inference time on 140M : 3 min on 40 x 8vCPU
- Performance of one HPU : 30% faster
- 200 identified molecules will be tested by MMV by the end of the year

Notices and Disclaimers
Performance varies by use, configuration, and other factors. Learn more at www.intel.com/PerformanceIndex. Performance results are based on testing as of dates shown in configurations and may not reflect all publicly available updates. No product or component can be absolutely secure. Your costs and results may vary. Intel technologies may require enabled hardware, software, or service activation.

© 2022, Amazon Web Services, Inc. or its affiliates. All rights reserved.

Thank you!

Learn more at Intel booth #1617



Please complete the session survey in the **mobile app**

© 2022, Amazon Web Services, Inc. or its affiliates. All rights reserved.