LFS305

Delivering life-changing medicines at AstraZeneca with data and AI

Anna Berg Åsberg
VP R&D IT
AstraZeneca

Chris Scott
Global Solutions Architect
AWS

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Agenda



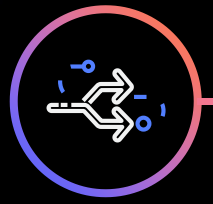
Delivering life-changing medicines at AstraZeneca



Architecture deep dive



Outcomes and lessons learned



What’s next and wrap-up

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Introducing AWS for Health

Accelerating innovation from benchtop to bedside

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Solutions across biopharma



Research and discovery

Clinical development

Manufacturing and supply chain

Commercial and medical affairs

Security and compliance

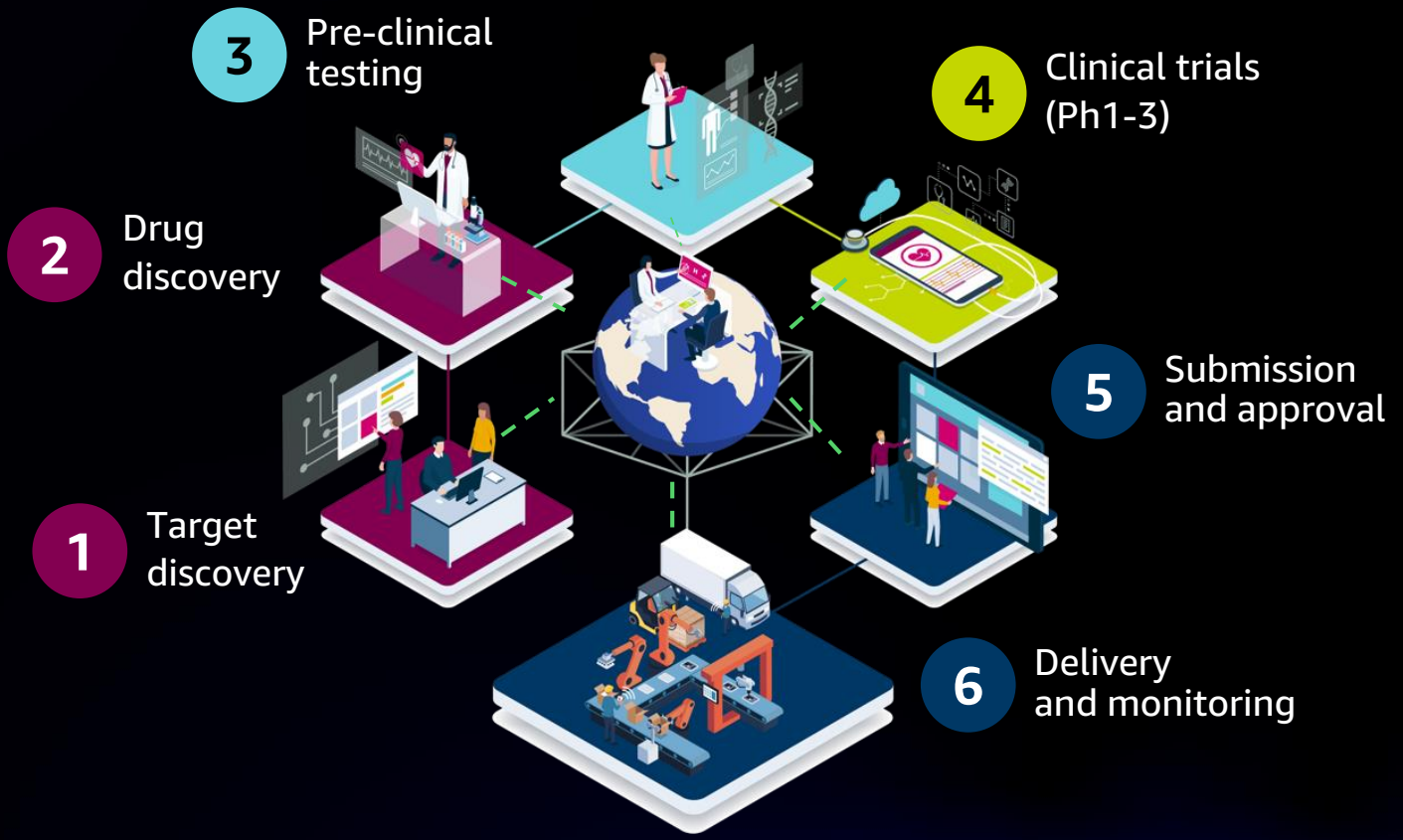
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Delivering life-changing medicines at AstraZeneca

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The role of R&D IT at AstraZeneca

Our purpose is to use technology to transform the speed and quality of the discovery and delivery of medicines to patients



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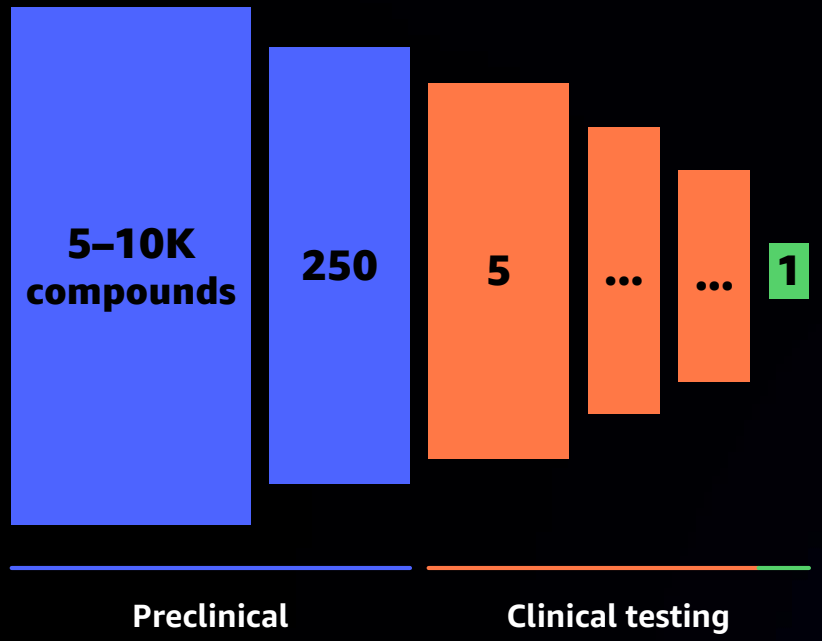
My story



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Biopharma R&D productivity and success rates are an industry-wide challenge

Can we make better decisions?



Can we develop new treatments faster?

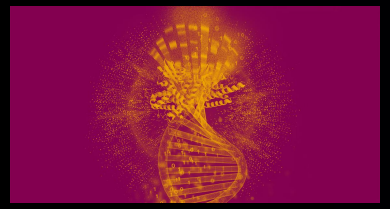


10+ years

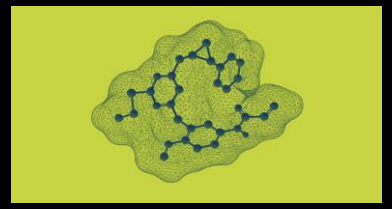
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Accelerating delivery of life-changing medicines by improving speed and accuracy with technology

Target discovery



Augmented drug design



Digital labs

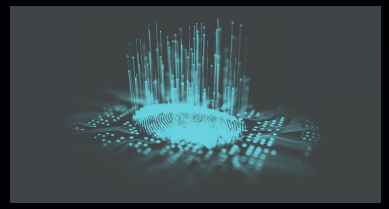
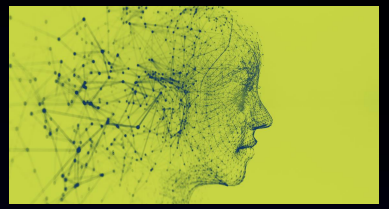




Image analysis



Tech in clinical trials



Natural language processing

aws

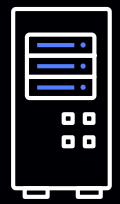
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Technical challenges



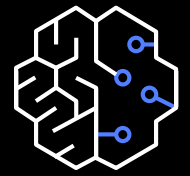
Data silos

1



Limited performance and capacity

2

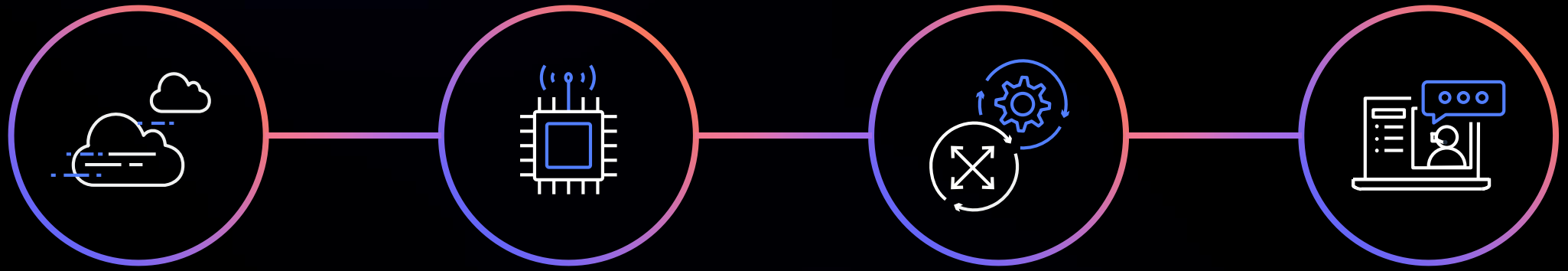


Limited use of AI/ML

3

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Why AWS?



Scale

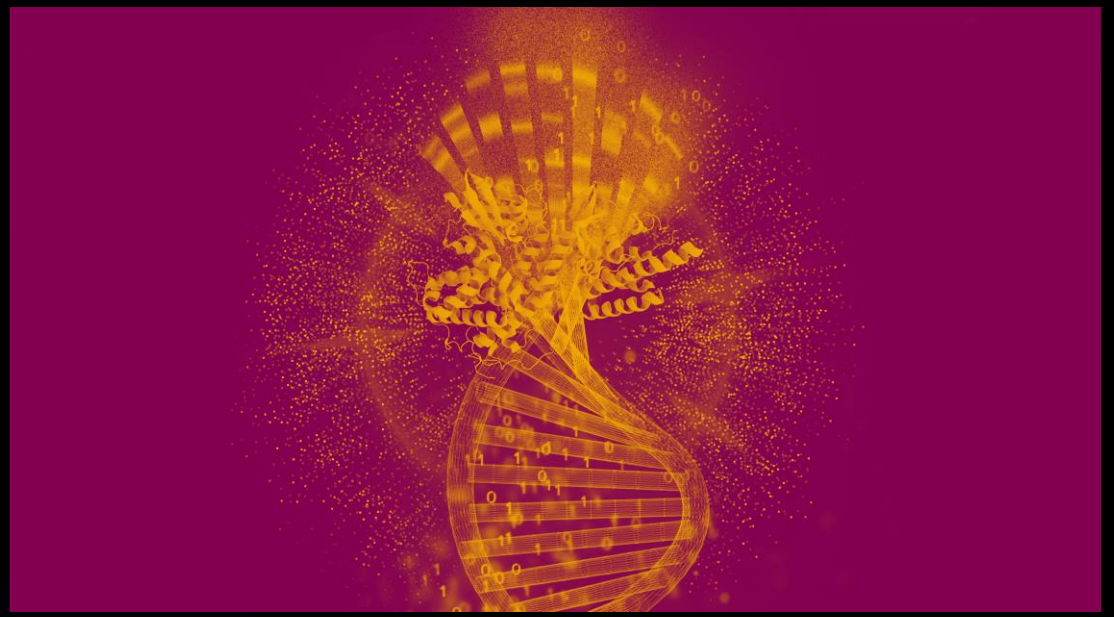
Compute power

Service offerings

Architecture guidance

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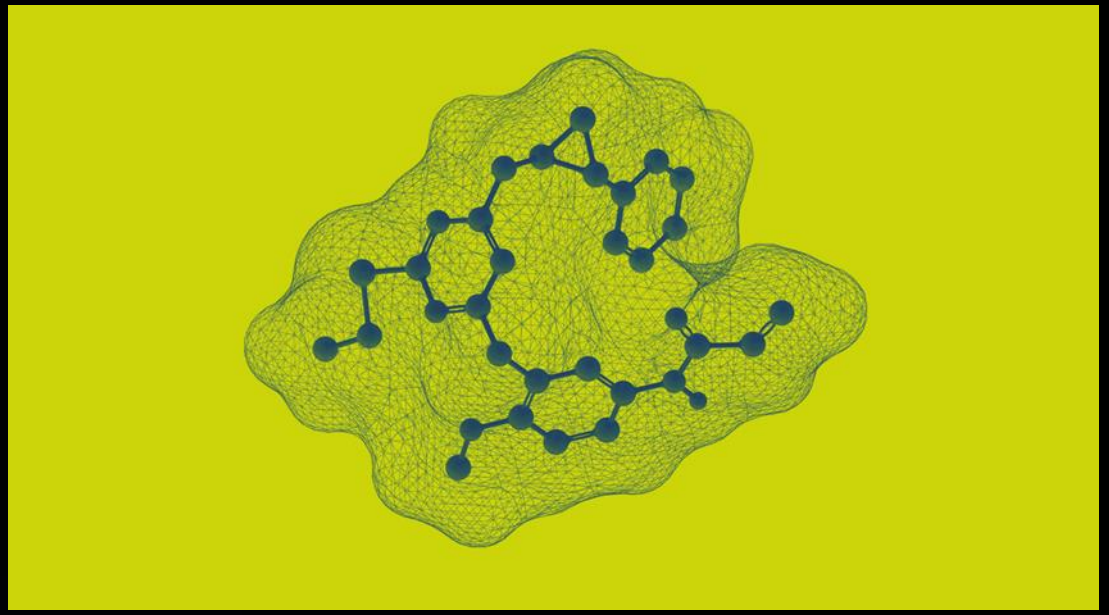
Target discovery: Handling explosion of data



Fast, efficient, cloud-based solution for extracting insights from the human genome

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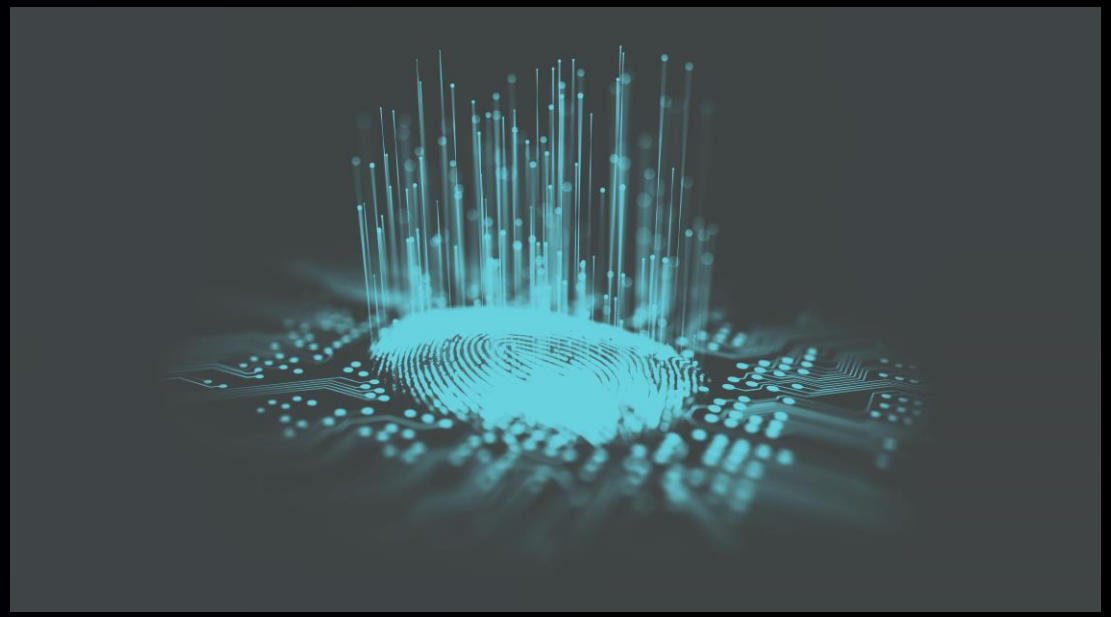
Drug discovery: Easy-to-use AI drives adoption



Augmented drug design to predict what molecules to make and how to make them

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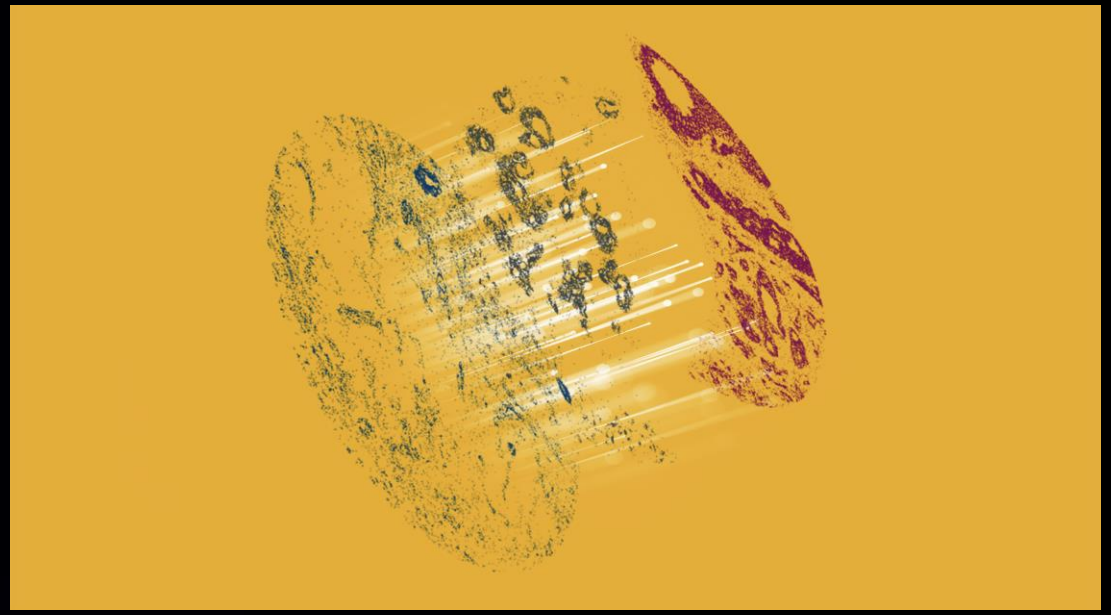
Digital labs: Digitizing scientists' workplaces



Modernized compute, optimized science apps, and data are captured at source and accessible remotely

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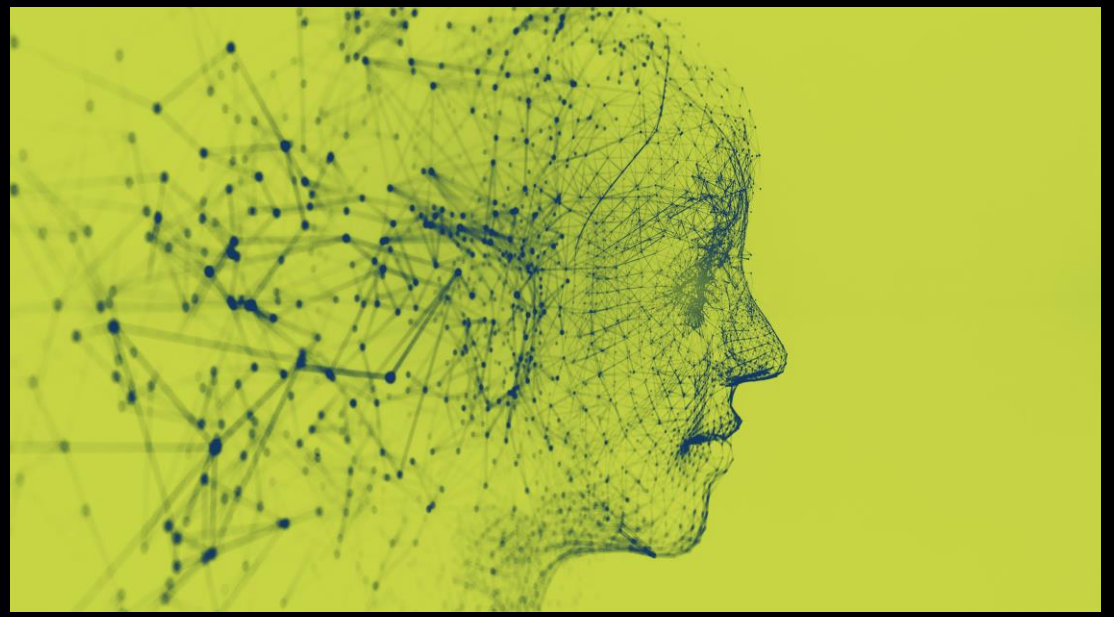
Preclinical testing: Using AI for fast, accurate image analysis



Annotating tumor images delivers new insights into patient types, research opportunities

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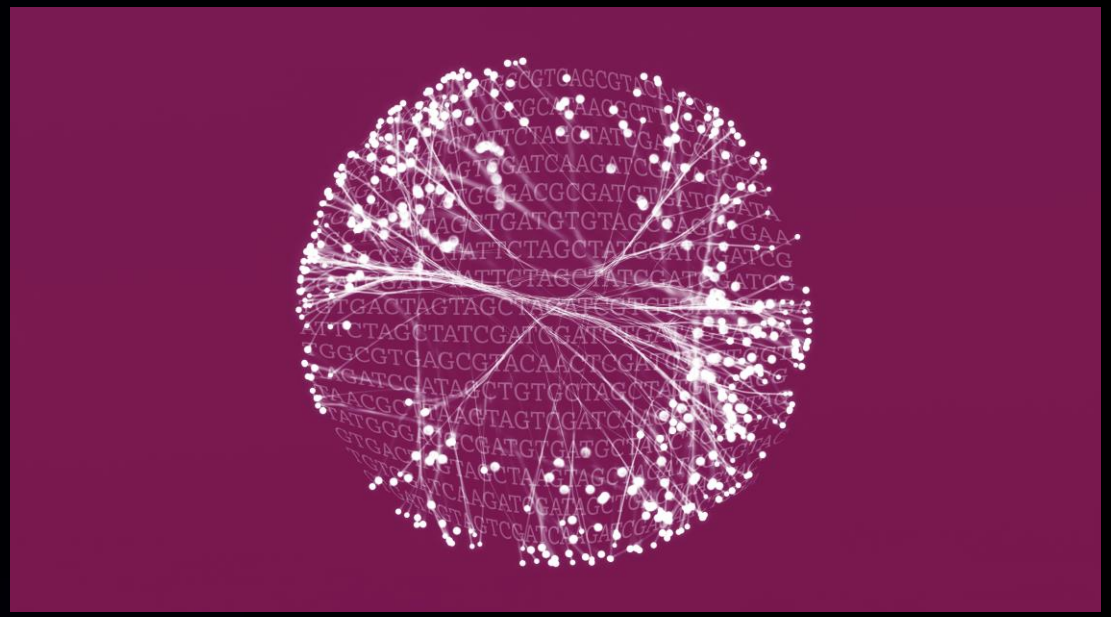
Clinical trials: Making frictionless experience for customers



Building cutting-edge technology to drive more efficient, patient-centric clinical trial programs

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Submission and approval, delivery and monitoring: Automating handling of customer feedback

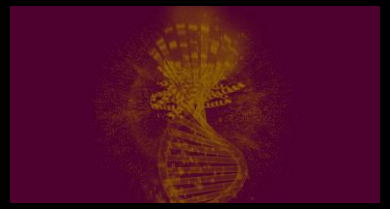


Simplifying our end-to-end clinical, regulatory and safety processes, applying NLP, deep learning, ML

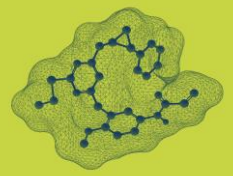
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Accelerating the delivery of life-changing medicines

Target discovery



Augmented drug design



Digital labs



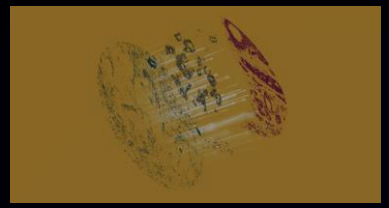


Image analysis



Tech in clinical trials



Natural language processing

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Architecture deep dive

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Unlocking and accessing chemistry data



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Architecture tenets

Managed services



Microservices-based architecture



Open source

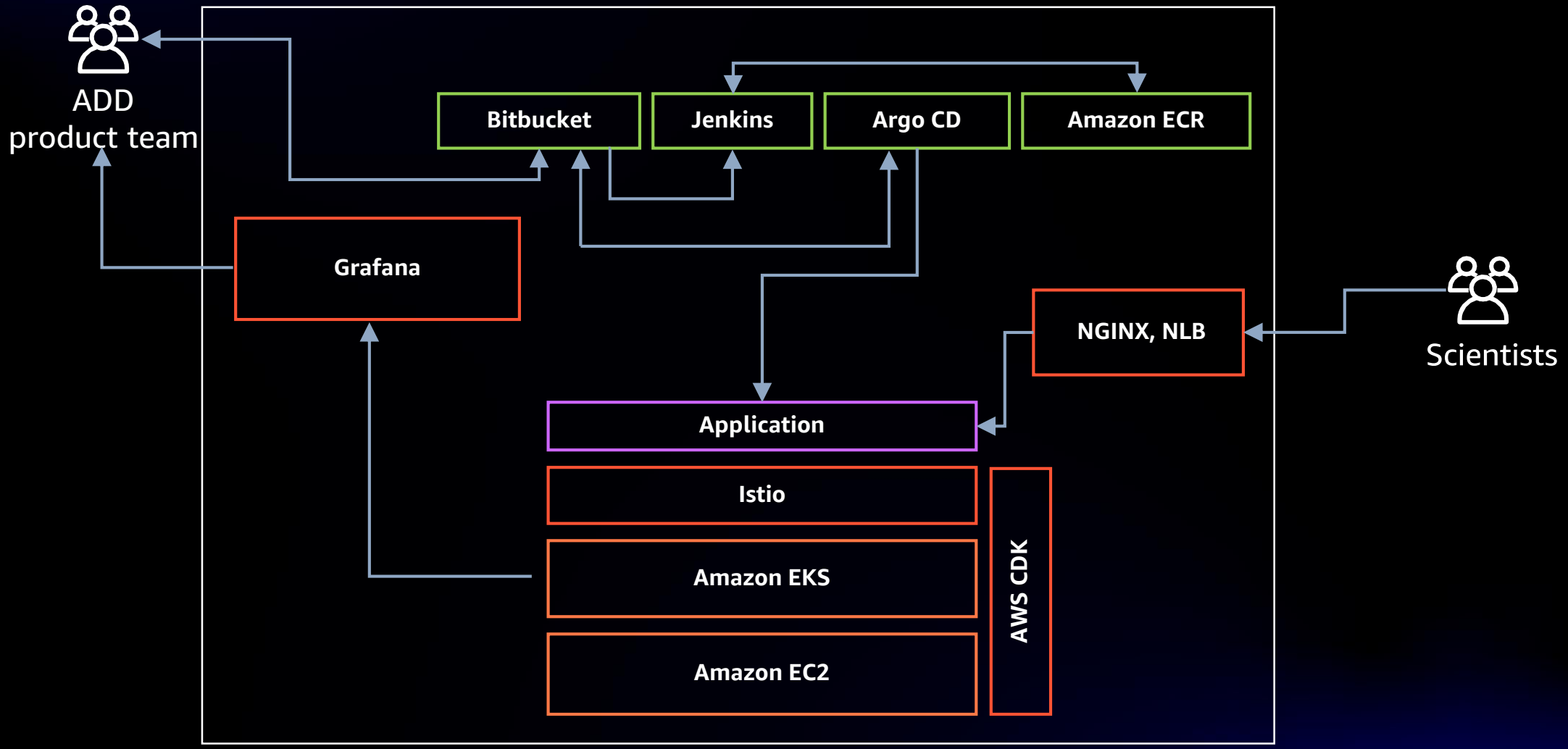


Infrastructure as code



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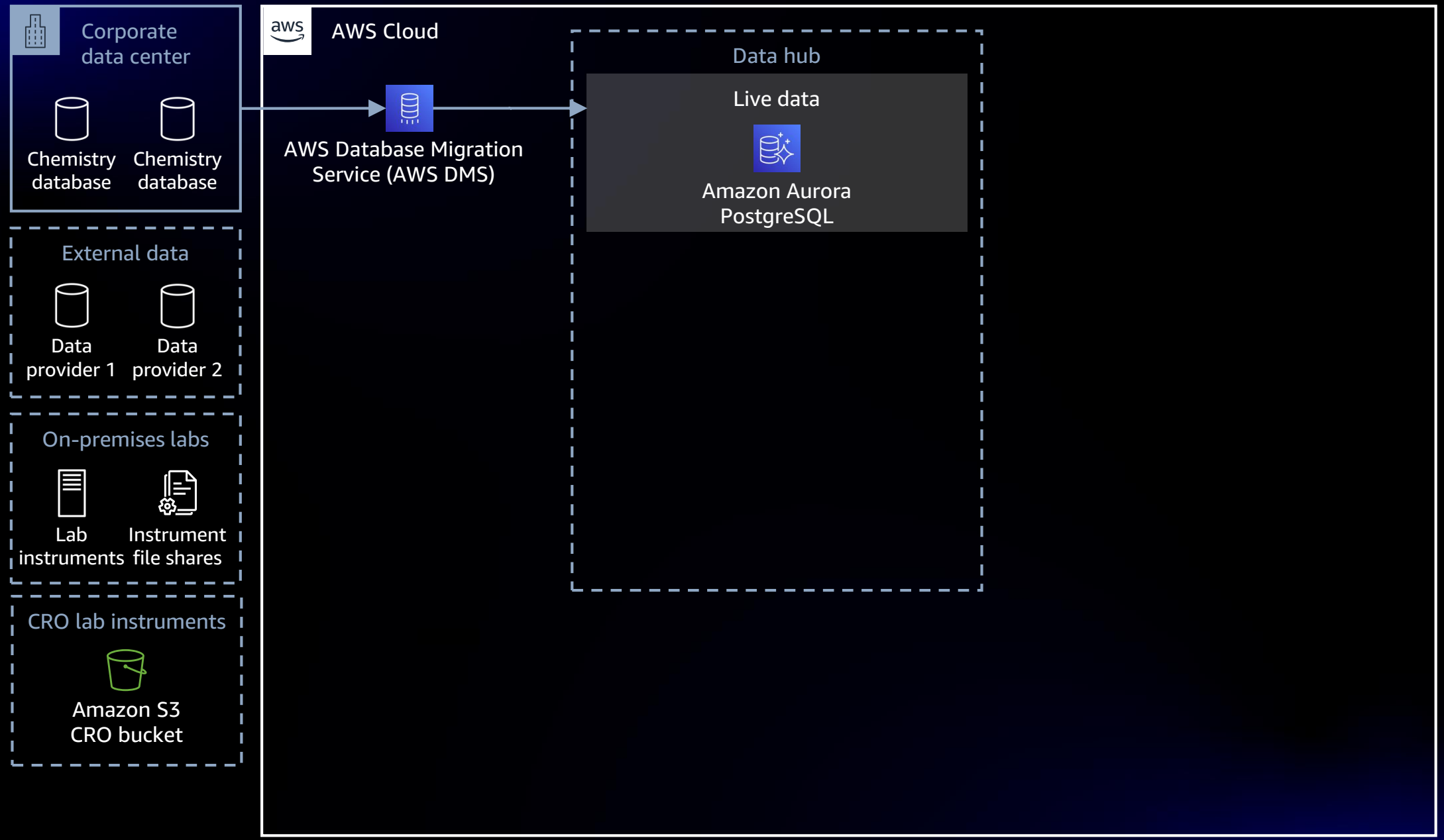
Amazon EKS – Open flexibility



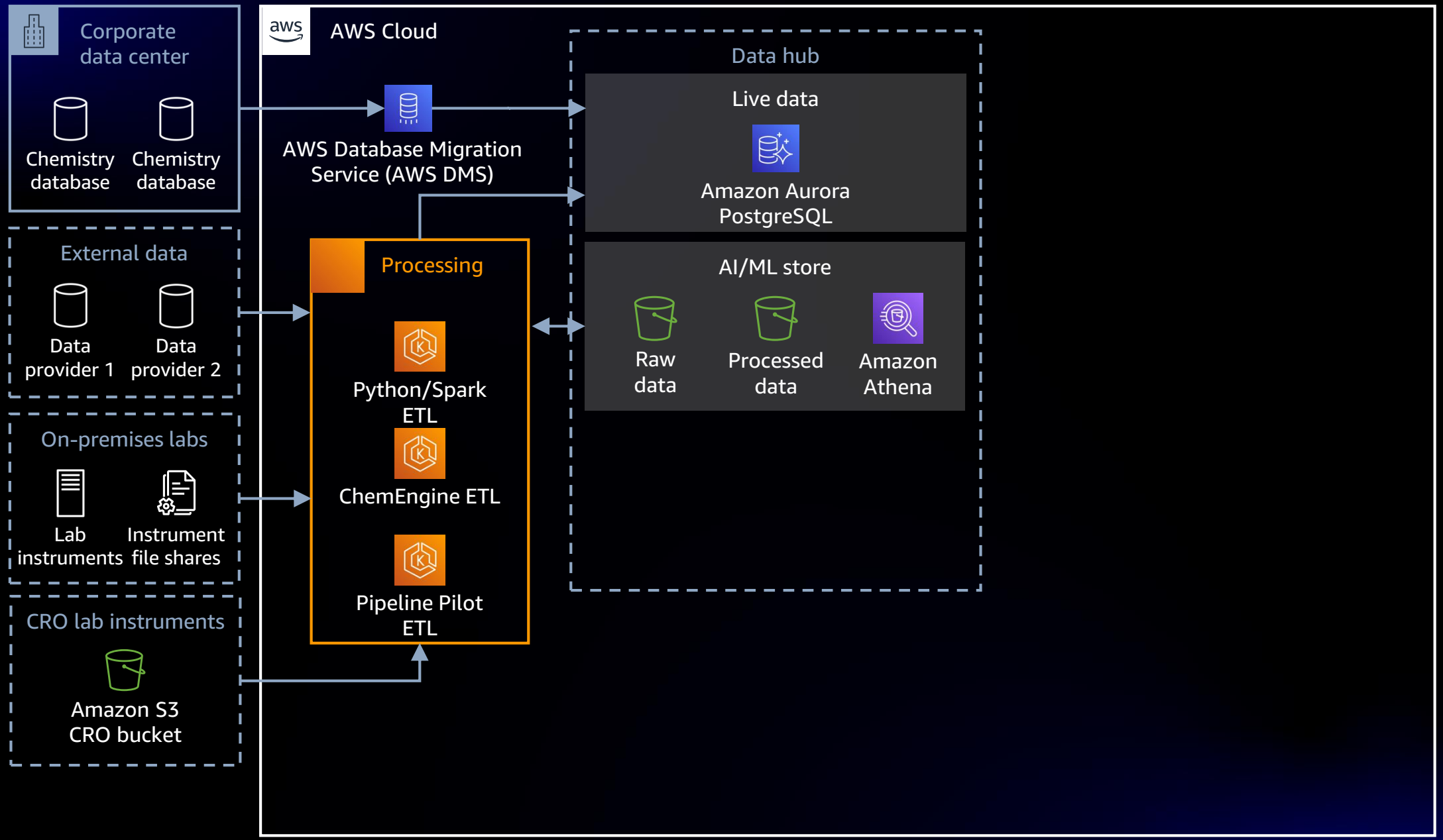
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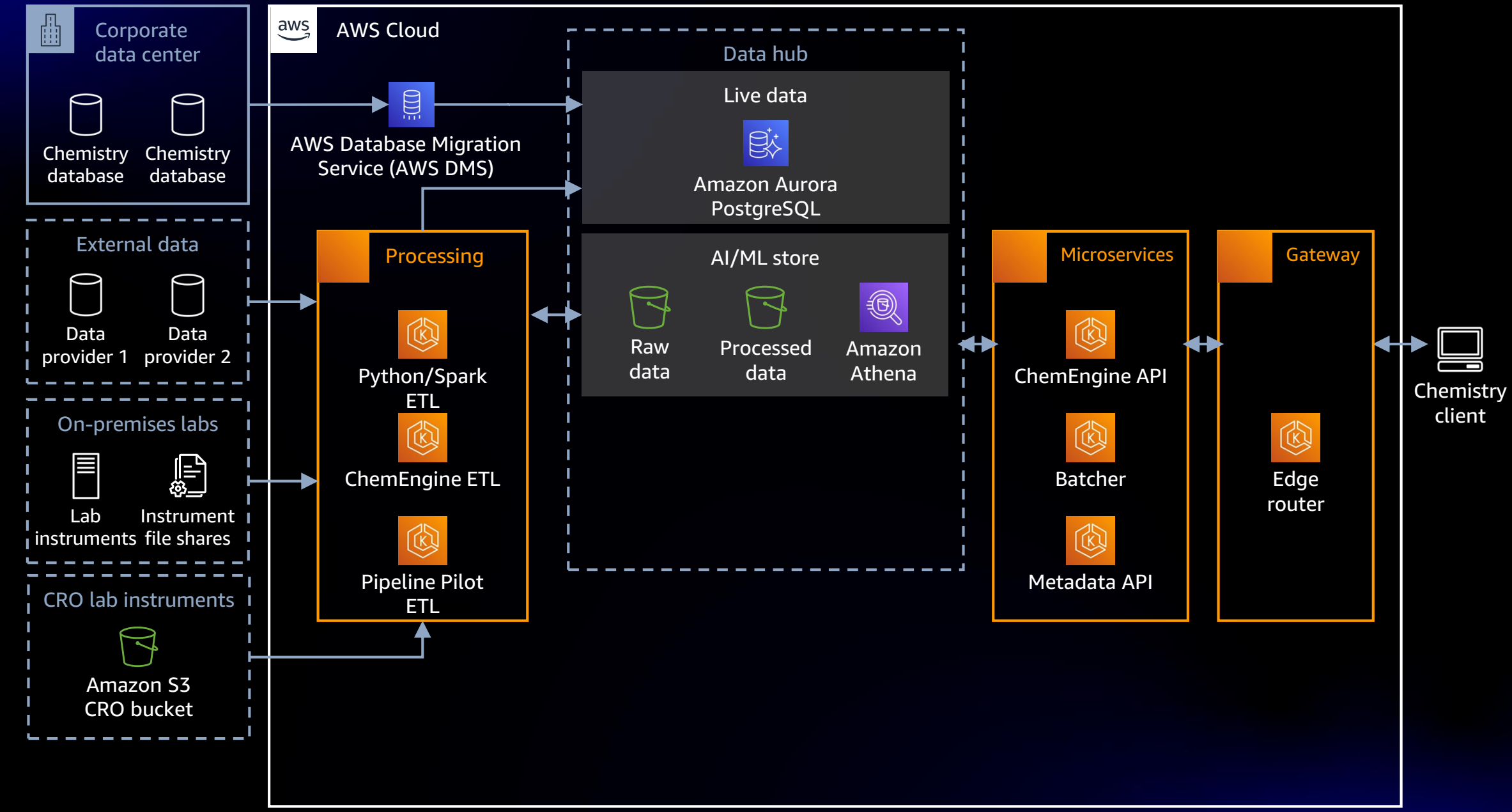
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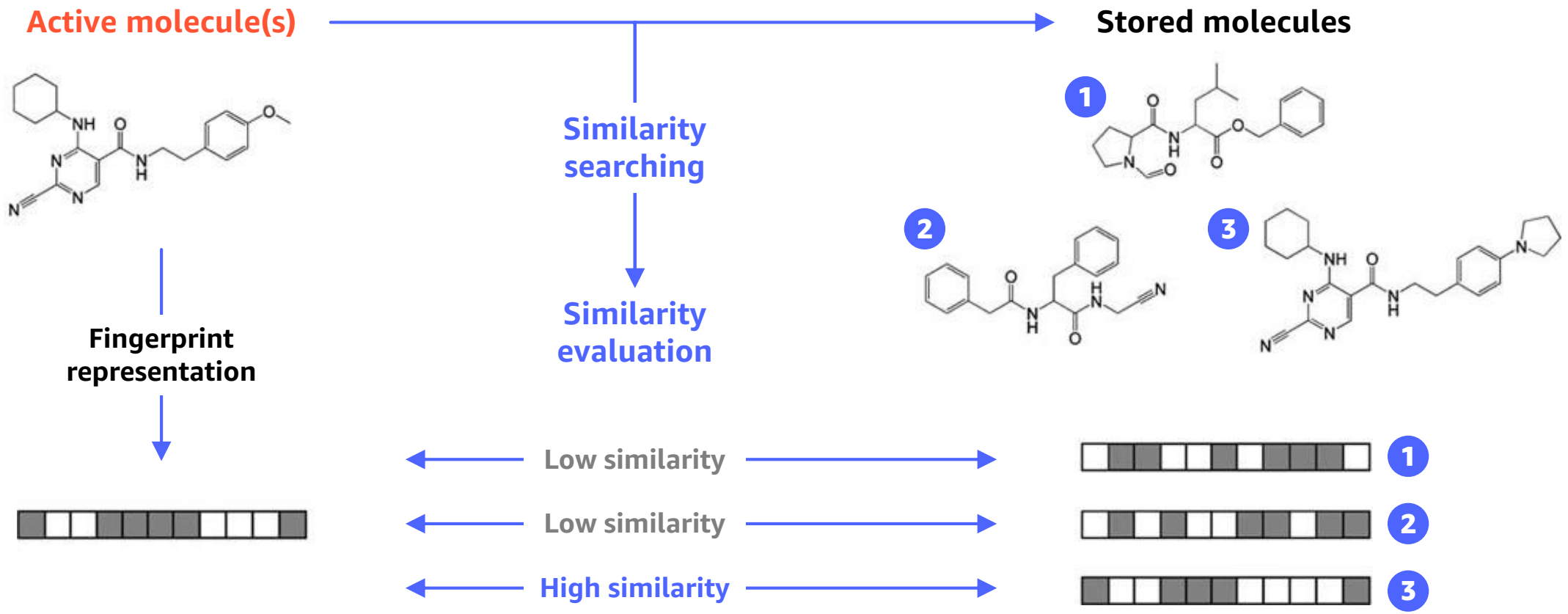


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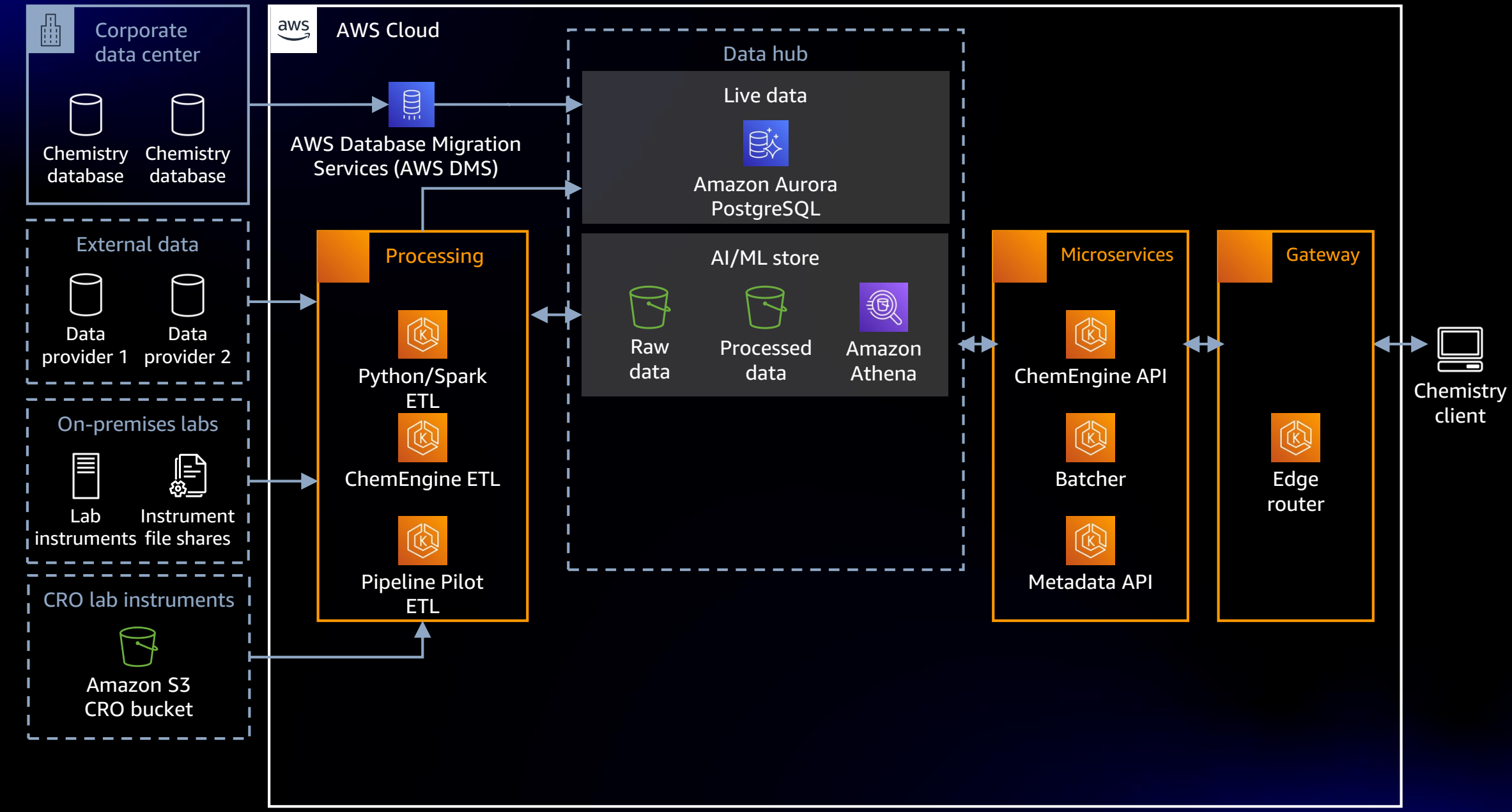


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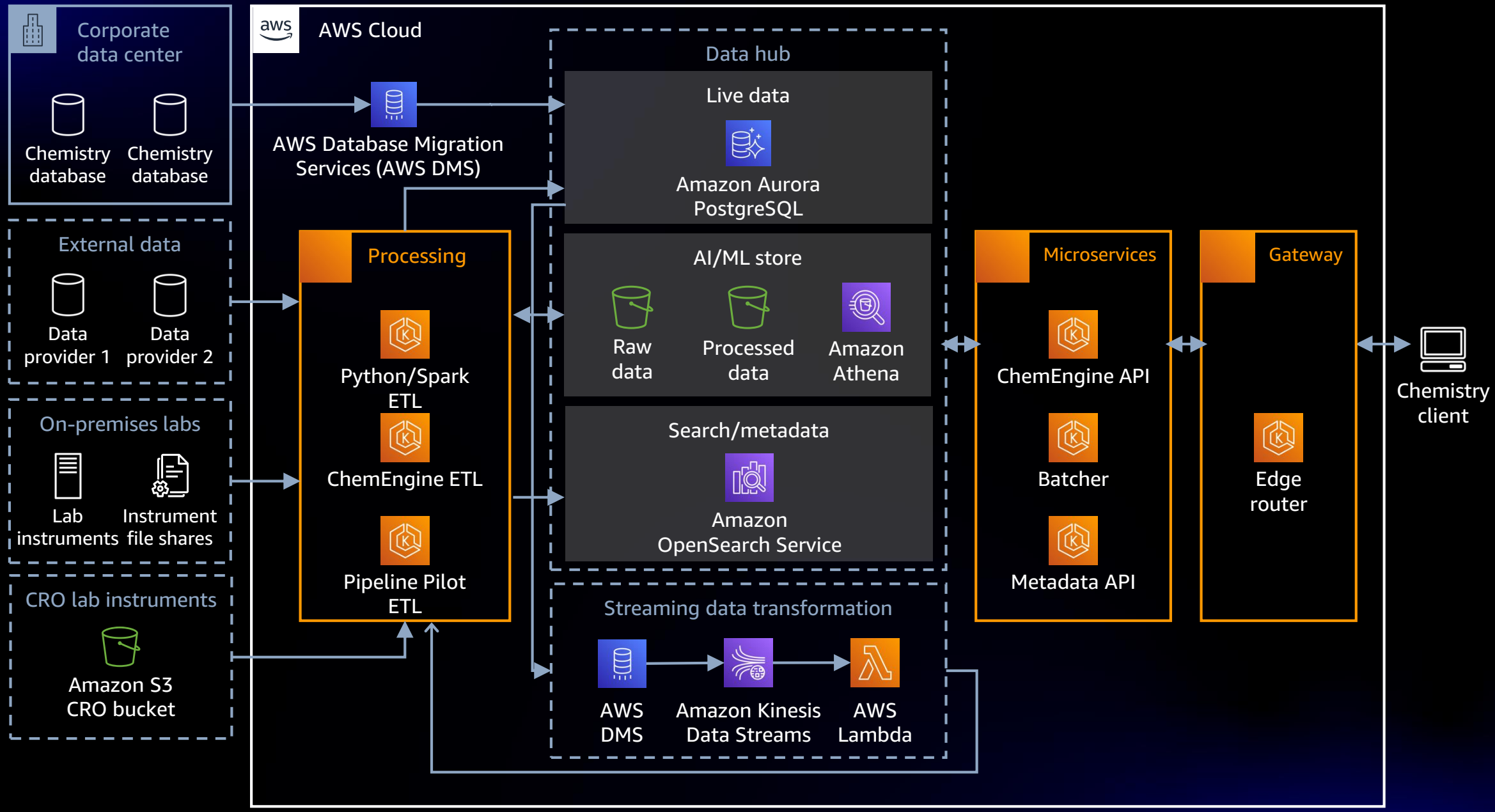
Molecular fingerprint search



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Data – Foundational building block



Unlock data silos

Advanced chemistry search

Scalable application gateway

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Drug discovery

Lead identification

Lead optimization

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Drug discovery



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Drug discovery

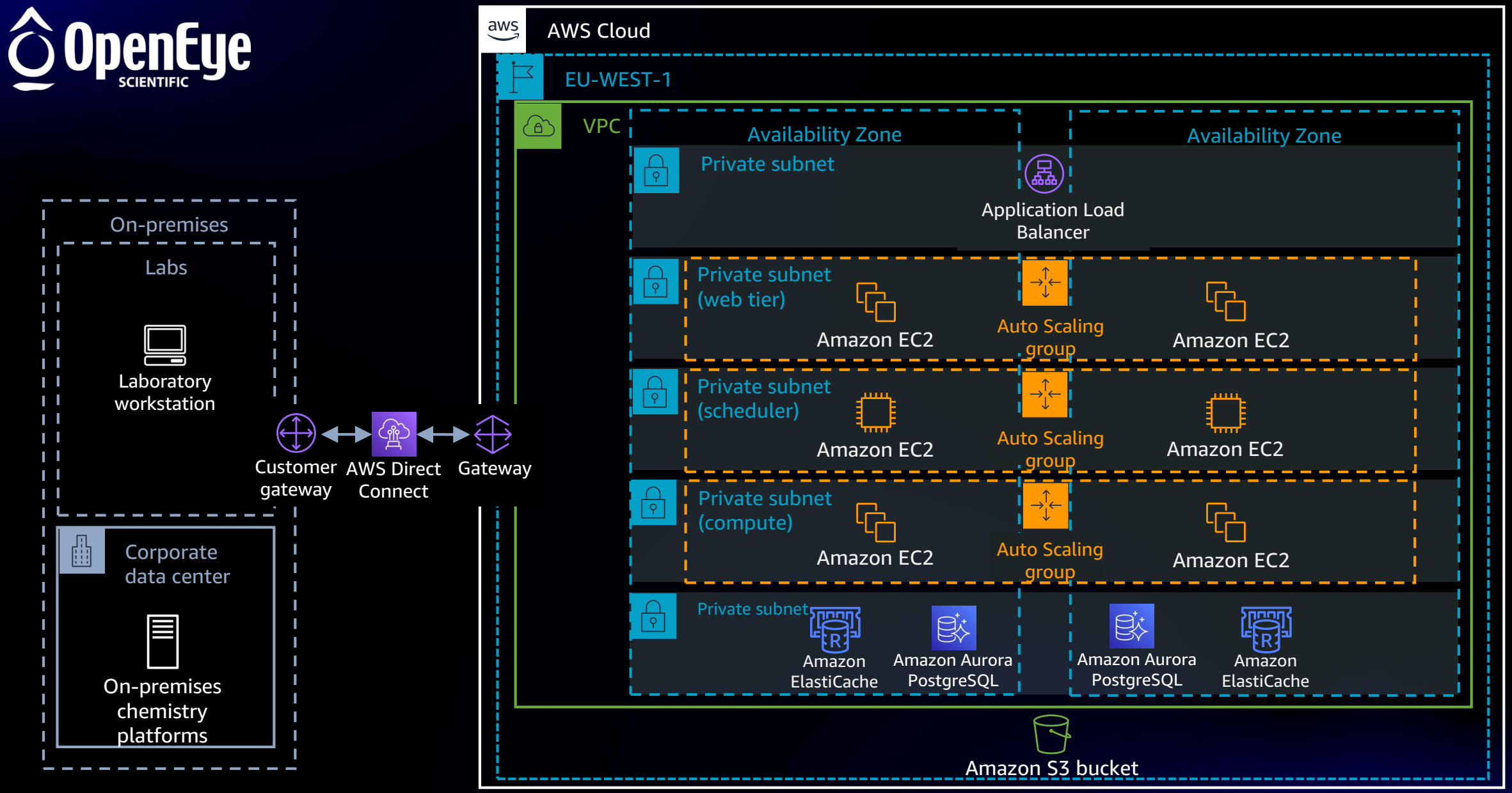


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Drug discovery



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Virtual screening at scale



Improved lead identification

1



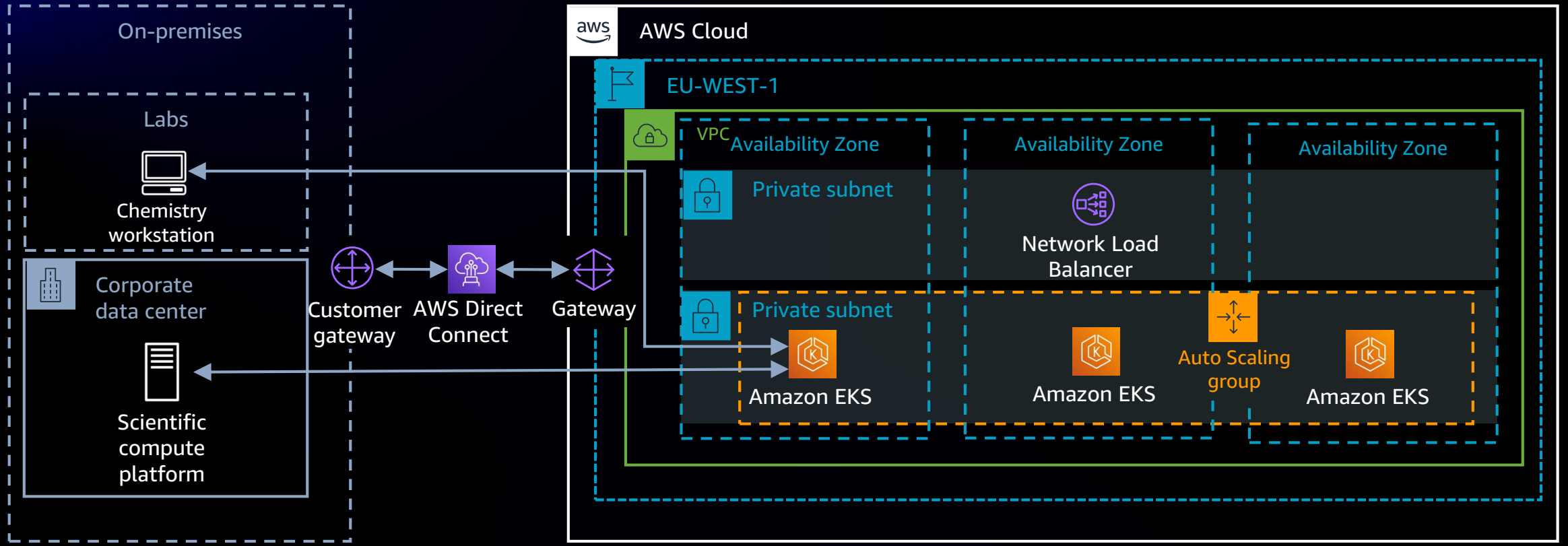
Speed and scale

2

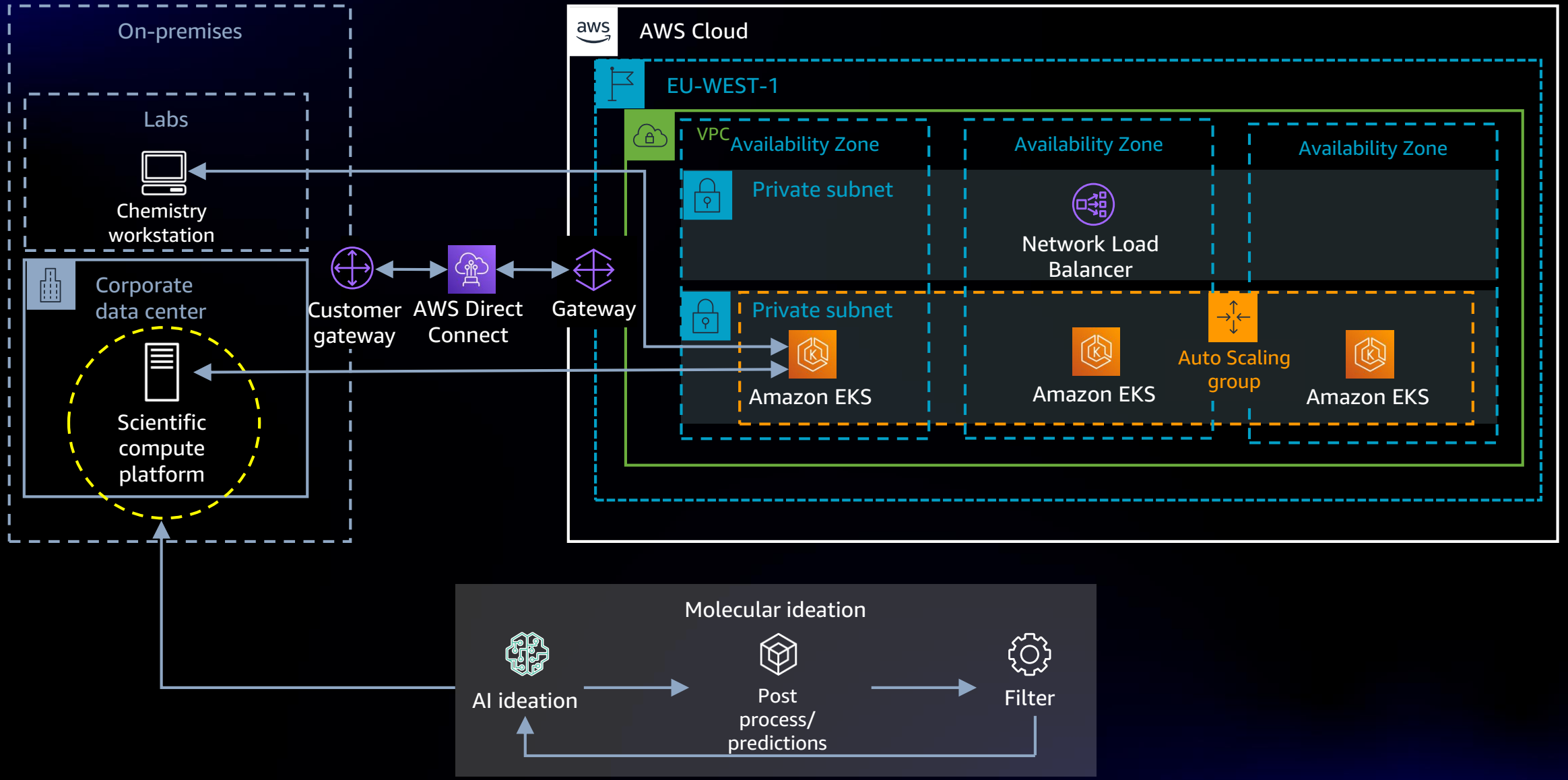
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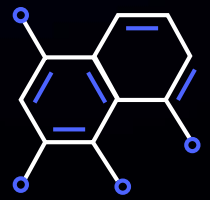


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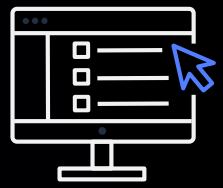
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AI ideation benefits



Acceleration of new molecule ideas

1



Common API control plane

2

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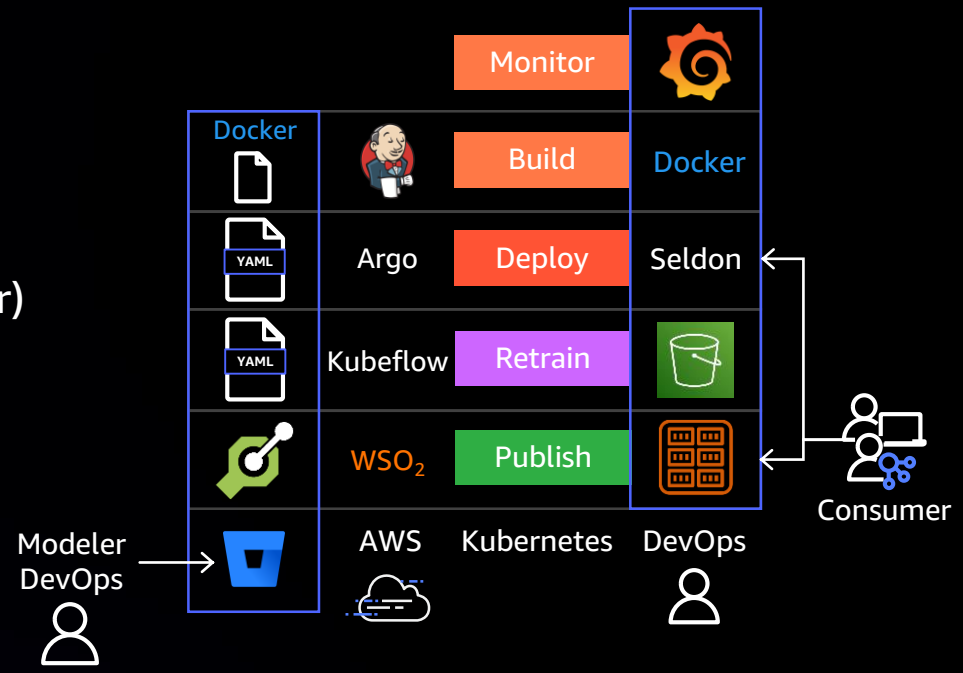
Predictive insights platform

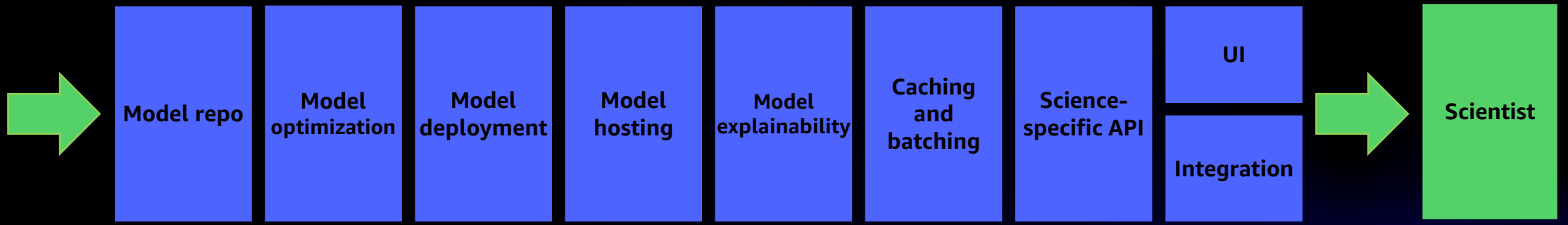
SCOPE

- Scalable predictive platform for all drug discovery
- Load models in less than a day

MODEL SOURCE

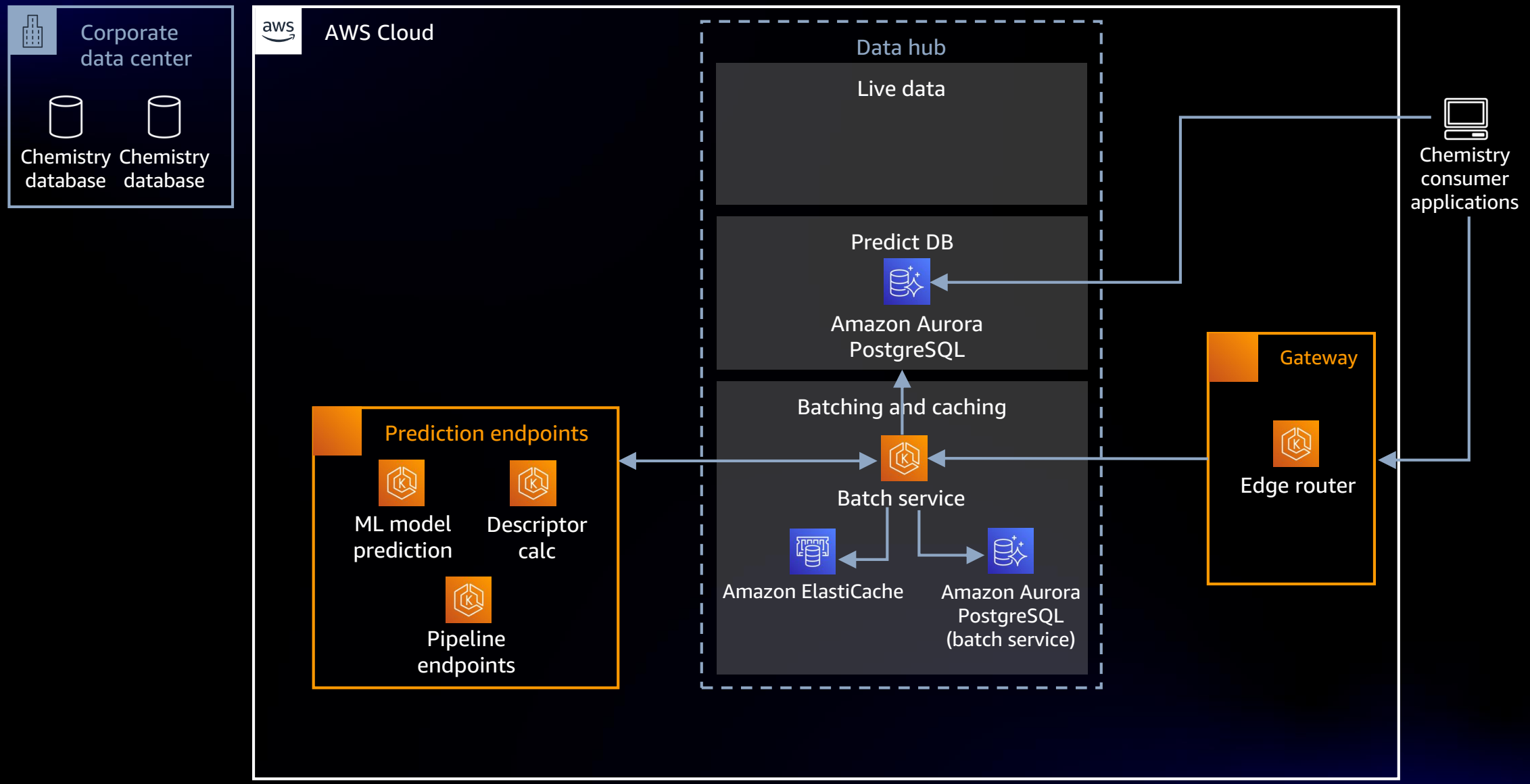
- SCP – AstraZeneca HPC
- GPU workstations
- AI Bench (Amazon SageMaker)
- MELLODDY consortium
- NVIDIA Cambridge 1



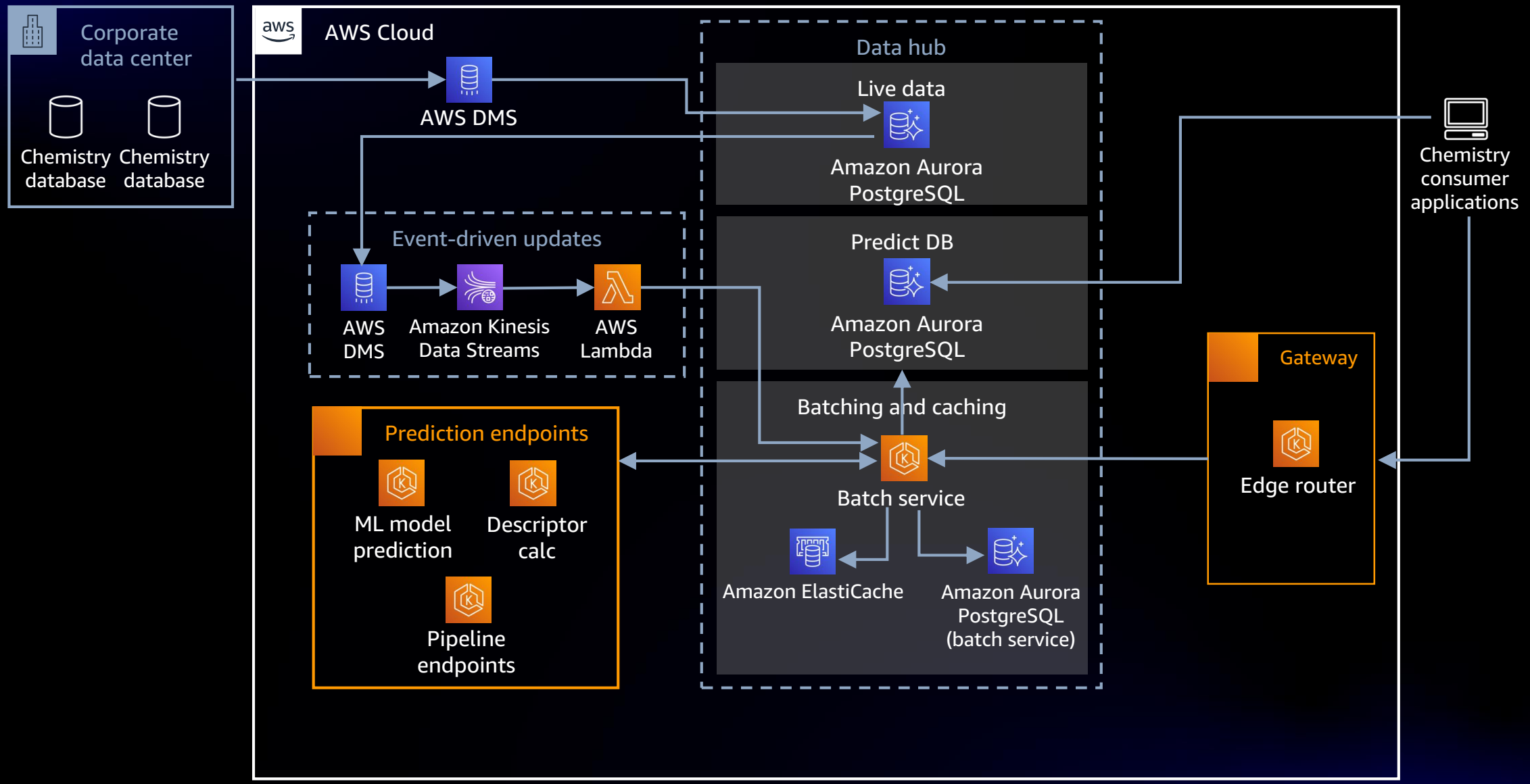


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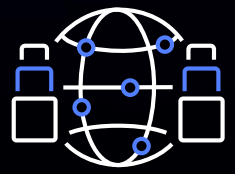


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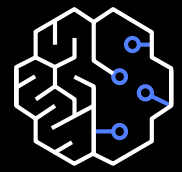
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Predictive insights platform value



Millions of predictions

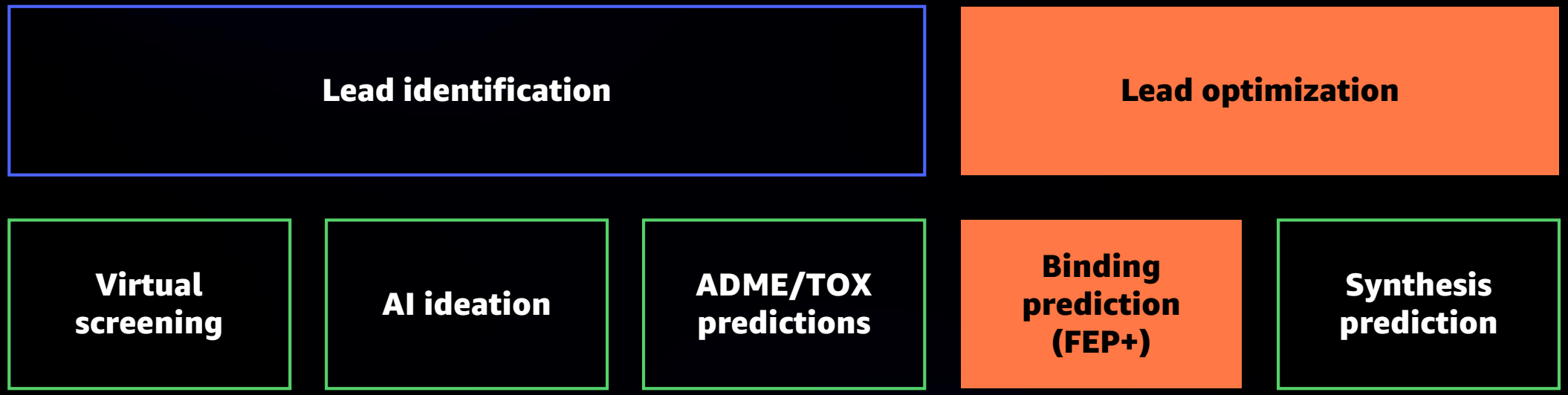
1



Accelerated model deployment

2

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aws

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FEP+ challenges



Improve binding accuracy

1



Limited performance and capacity

2

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Schrödinger FEP+: Enter the GPU



Amazon EC2

- Up to 8 NVIDIA Tesla V100 GPUs, each pairing 5,120 CUDA Cores and 640 Tensor Cores
- High-frequency Intel Xeon E5-2686 v4 (Broadwell) processors for p3.2xlarge, p3.8xlarge, and p3.16xlarge, and 2.5 GHz (base) Intel Xeon 8175M processors for p3dn.24xlarge
- Provides up to 100 Gbps of aggregate network bandwidth

aws

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Schrödinger FEP+: Enter the GPU



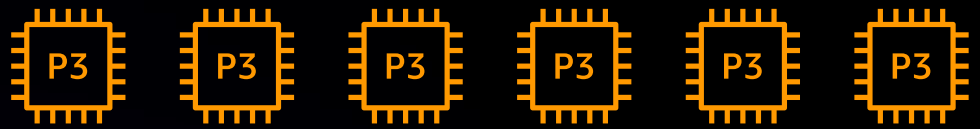
Amazon EC2

- Up to 8 NVIDIA Tesla V100 GPUs, each pairing 5,120 CUDA Cores and 640 Tensor Cores
- High-frequency Intel Xeon E5-2686 v4 (Broadwell) processors for p3.2xlarge, p3.8xlarge, and p3.16xlarge, and 2.5 GHz (base) Intel Xeon 8175M processors for p3dn.24xlarge
- Provides up to 100 Gbps of aggregate network bandwidth

Potential drug molecules



FEP+ active learning



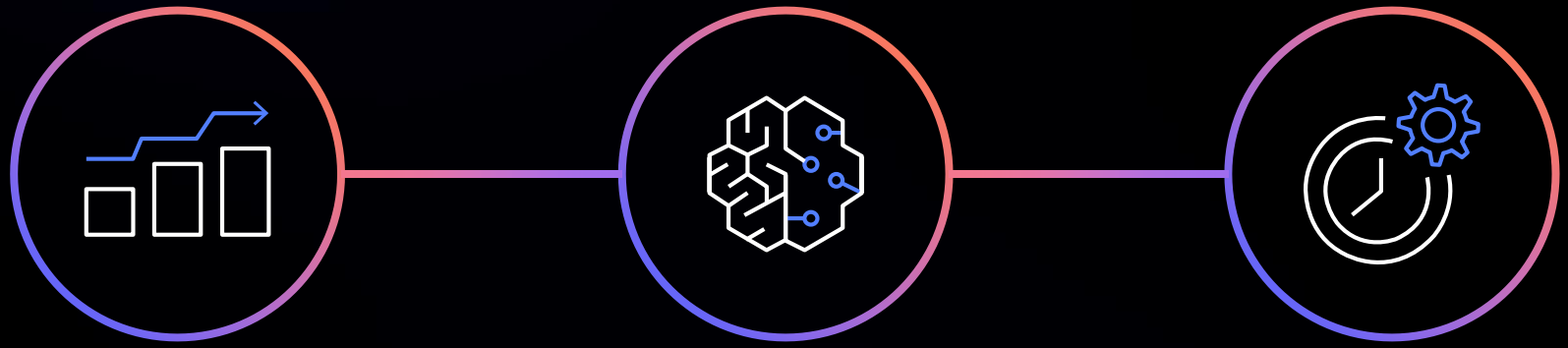


Circa 300,000 FEP+ calculations per annum

aws

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Schrödinger FEP+ outcomes



Increased accuracy

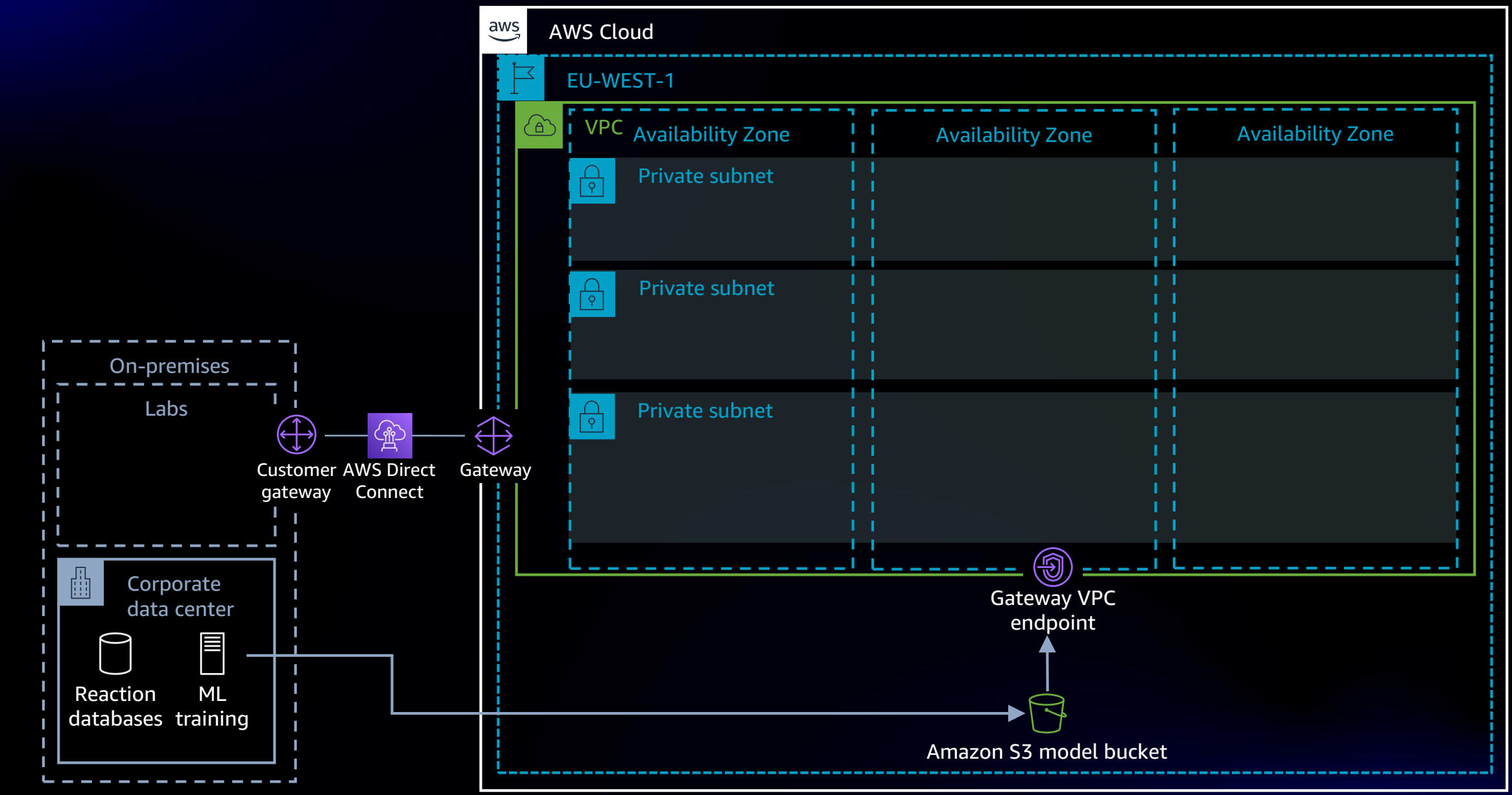
Continuously trained model

Scaled-out GPU compute

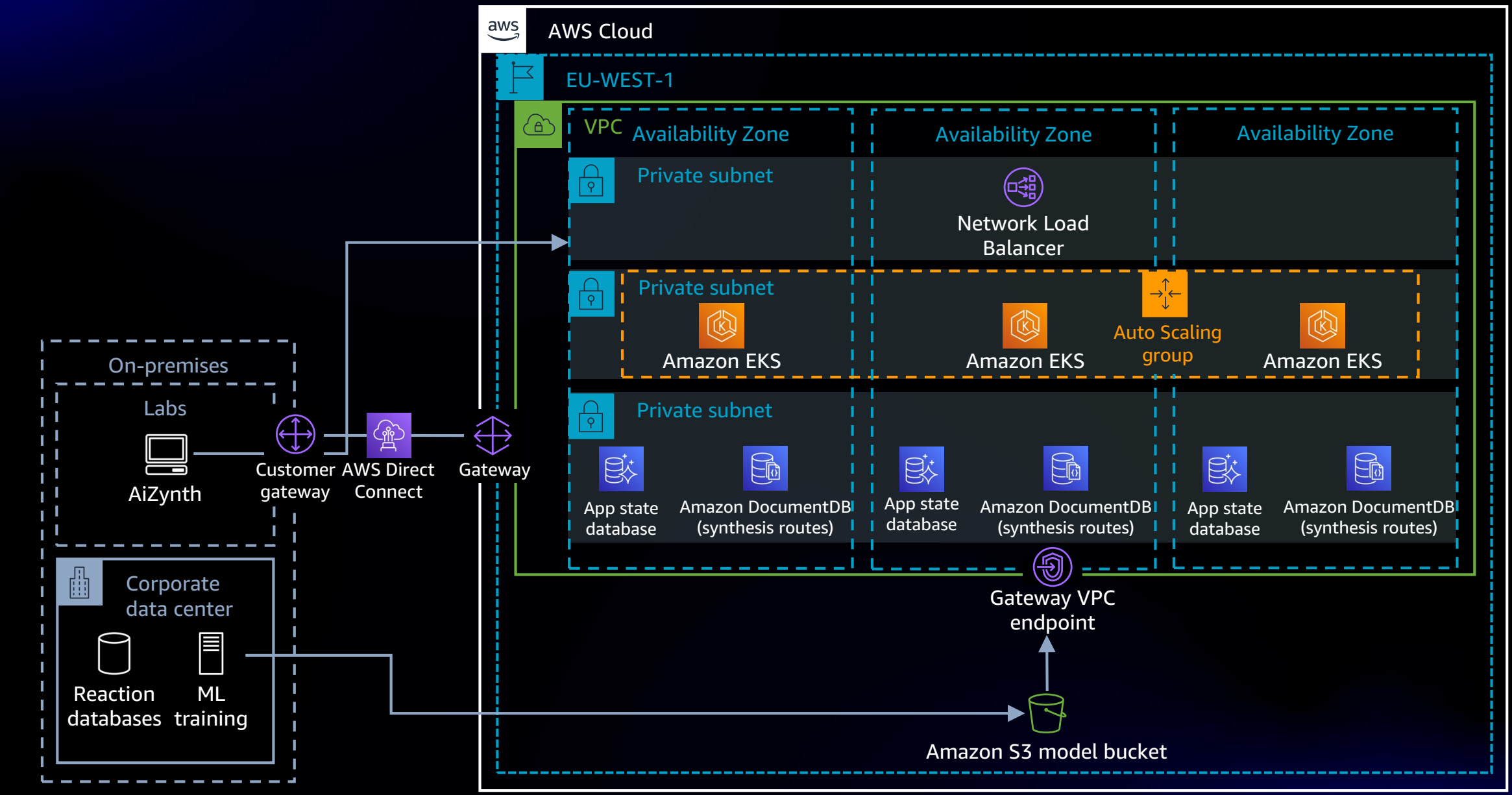
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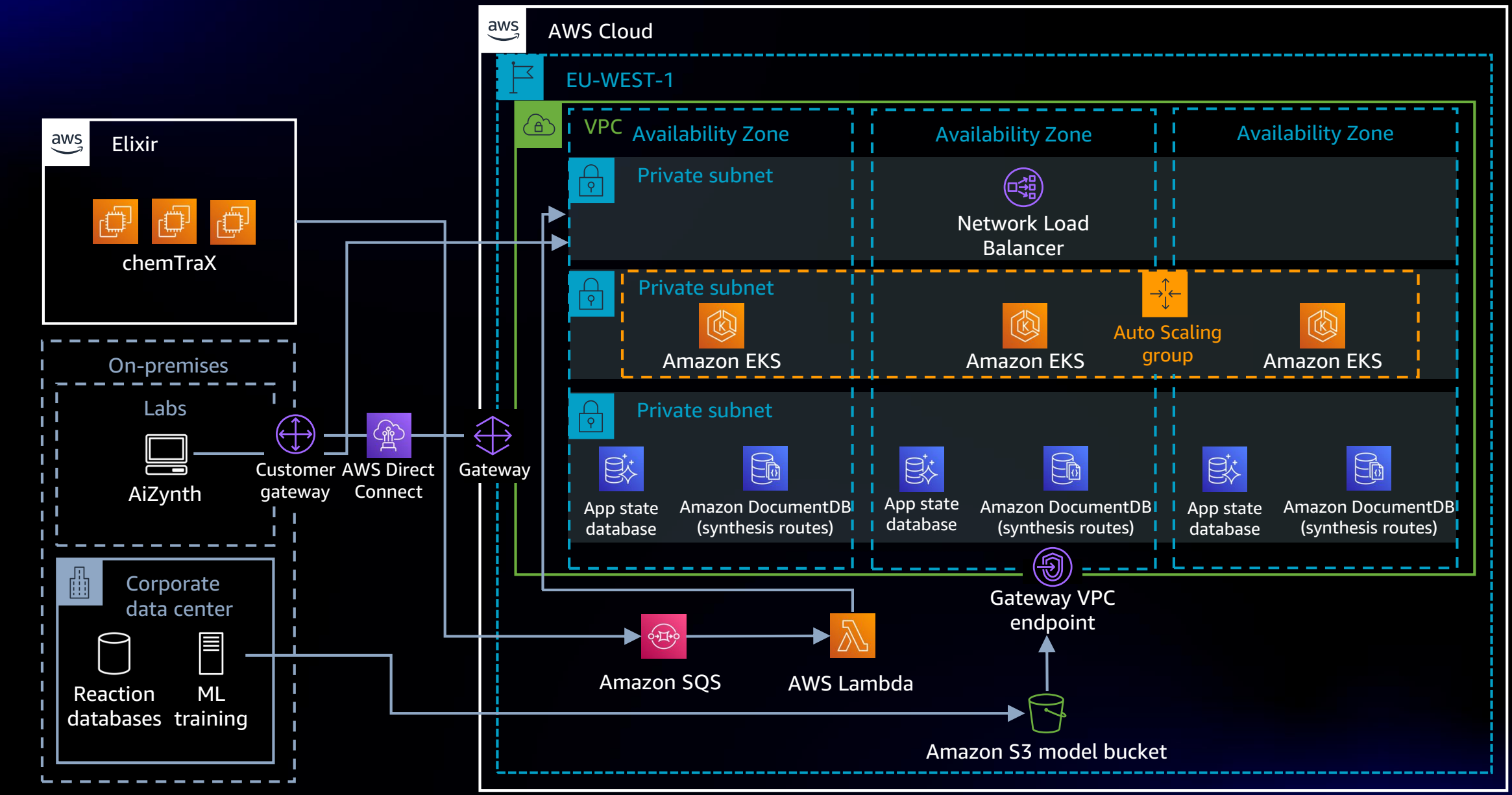
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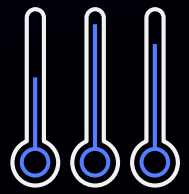


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Saving scientists’ time



Improved synthesis predictions

1



Saving laboratory time

2

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Let’s do some chemistry

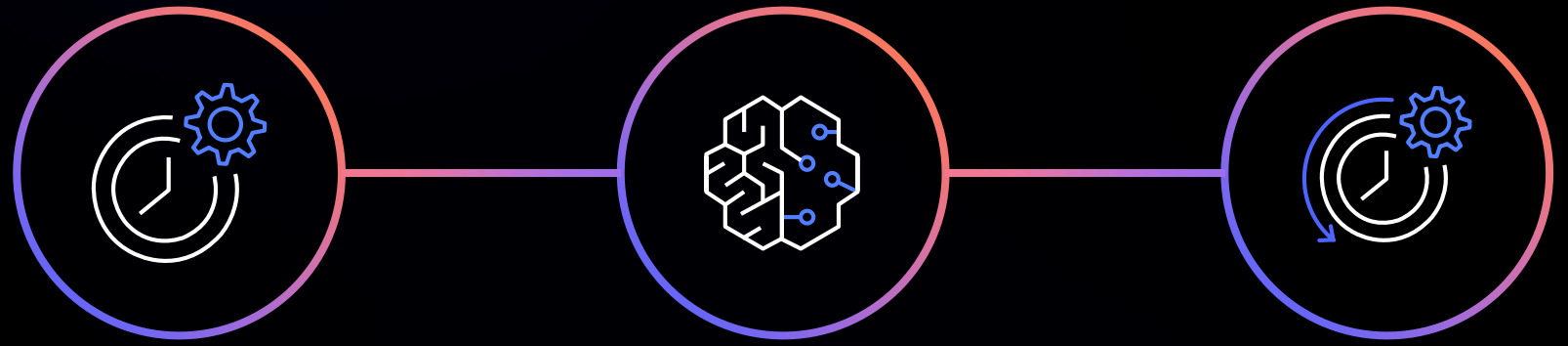


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Outcomes, lessons learned, and what's next

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Outcomes



Significant reduction in drug discovery time

Over 200 hosted data and AI endpoints

Model deployment down to less than 24 hours

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Lessons learned



Shared vision

1



Product-focused teams

2

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Next: Achieve new tech applications and scale to drive benefits



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Wrap-up



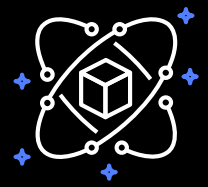
Modern architecture

1



Data and ML

2



AWS scalability, reliability, and availability

3

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Thank you!

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