Unify and accelerate AI drug discovery with Amazon Bio Discovery

From in-silico to wet-lab validated candidates in a single application

Case study: Agent guided de novo design of nanobody binders against a novel cancer target

Brenna McGahan, Applied Scientist at AWS AI Life Sciences
Fangda Xu, Applied Scientist at AWS AI Life Sciences

© 2026, Amazon Web Services, Inc. or its affiliates. All rights reserved. Amazon Confidential and Trademark.



Drug Discovery: Expensive and time consuming

10

years

$2.6

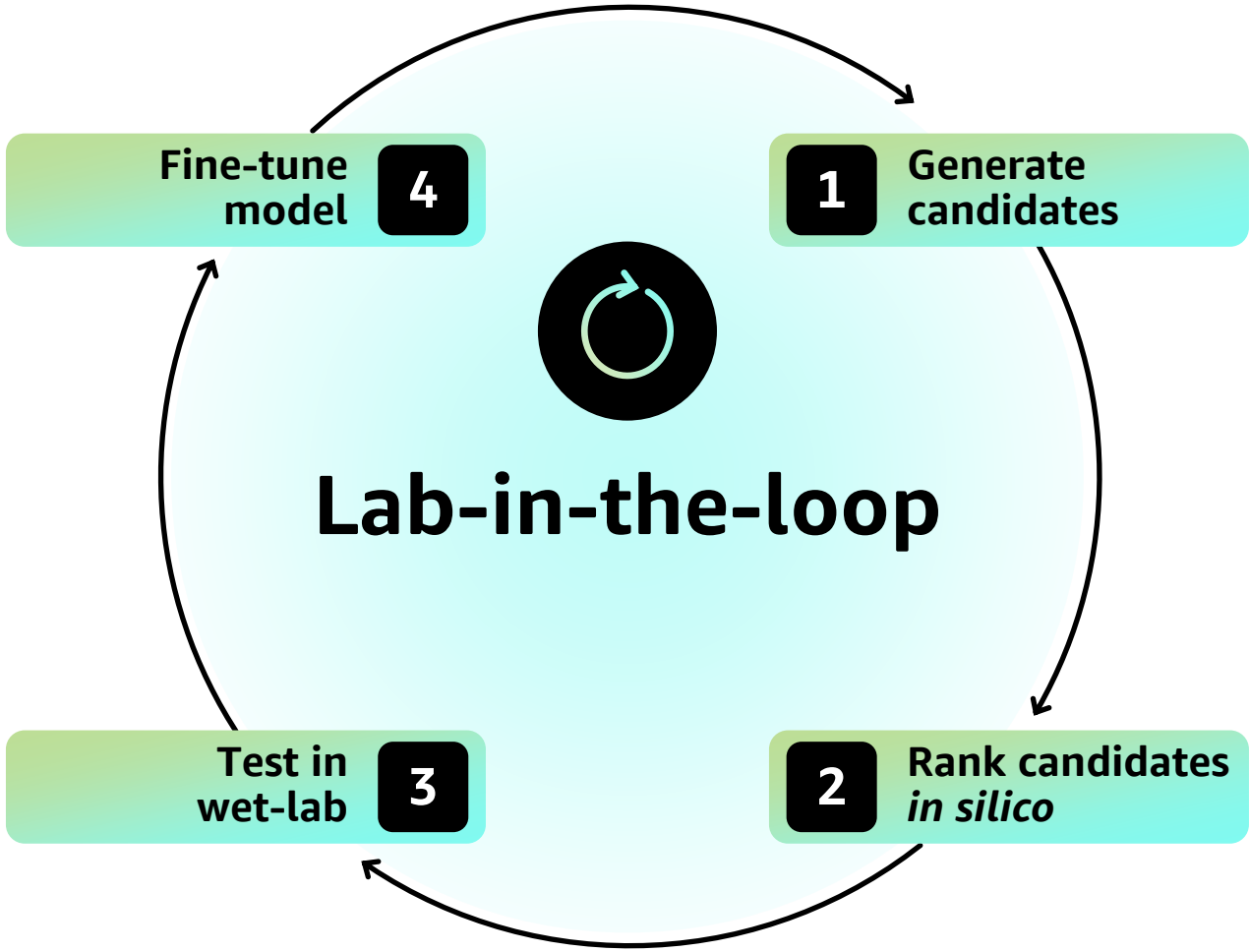
Billion dollars

BUT AI is cutting preclinical timelines from 3–4 years to **13–18 months**, with Phase I success rates nearly **doubling to 80–90%.**

© 2026, Amazon Web Services, Inc. or its affiliates. All rights reserved. Amazon Confidential and Trademark.

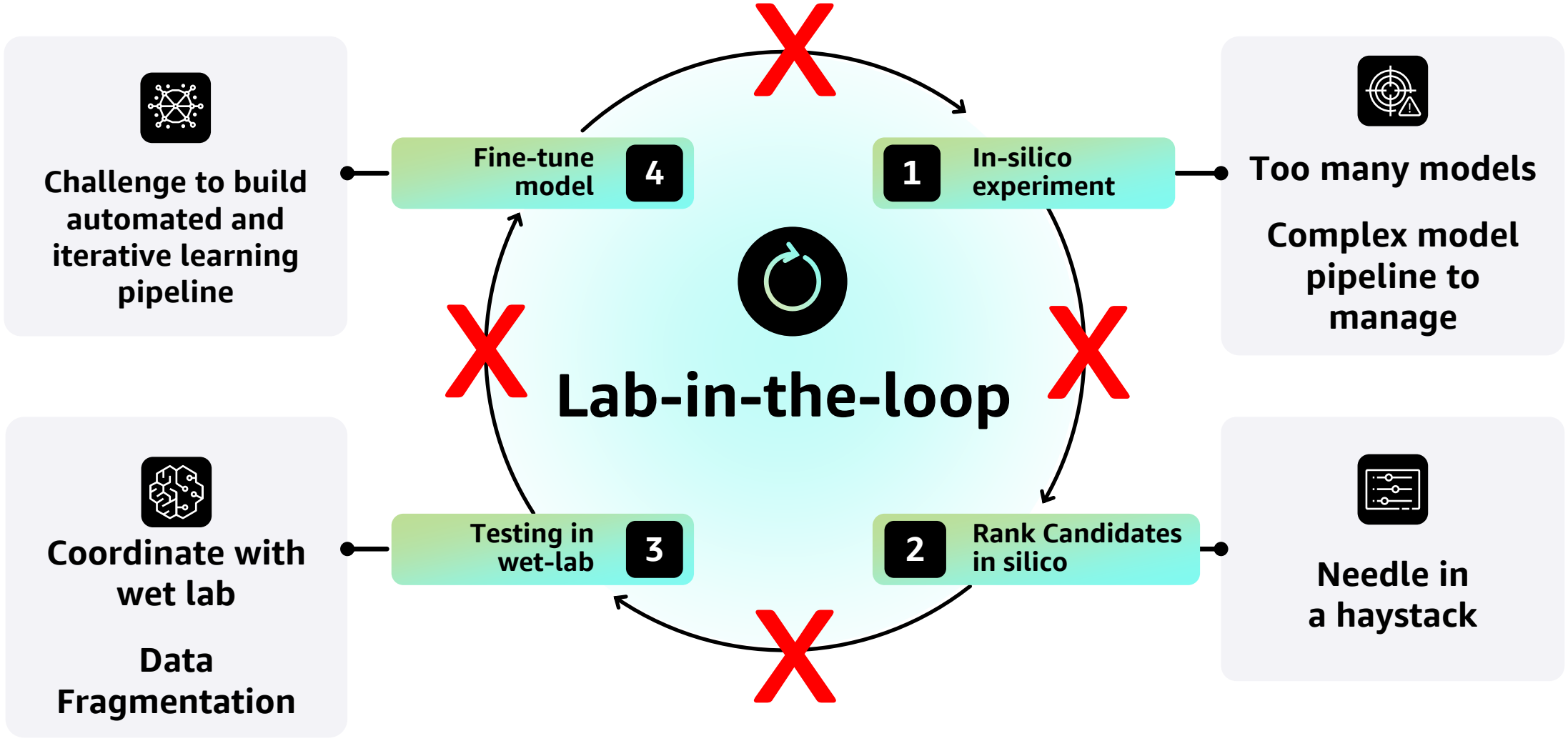
DiMasi et al., 2016
Fast Company (2016) - https://www.fastcompany.com/91520205/the-ai-drug-revolution-is-real-but-the-hype-around-it-isnt

Lab-in-the-Loop has the potential to transform drug discovery



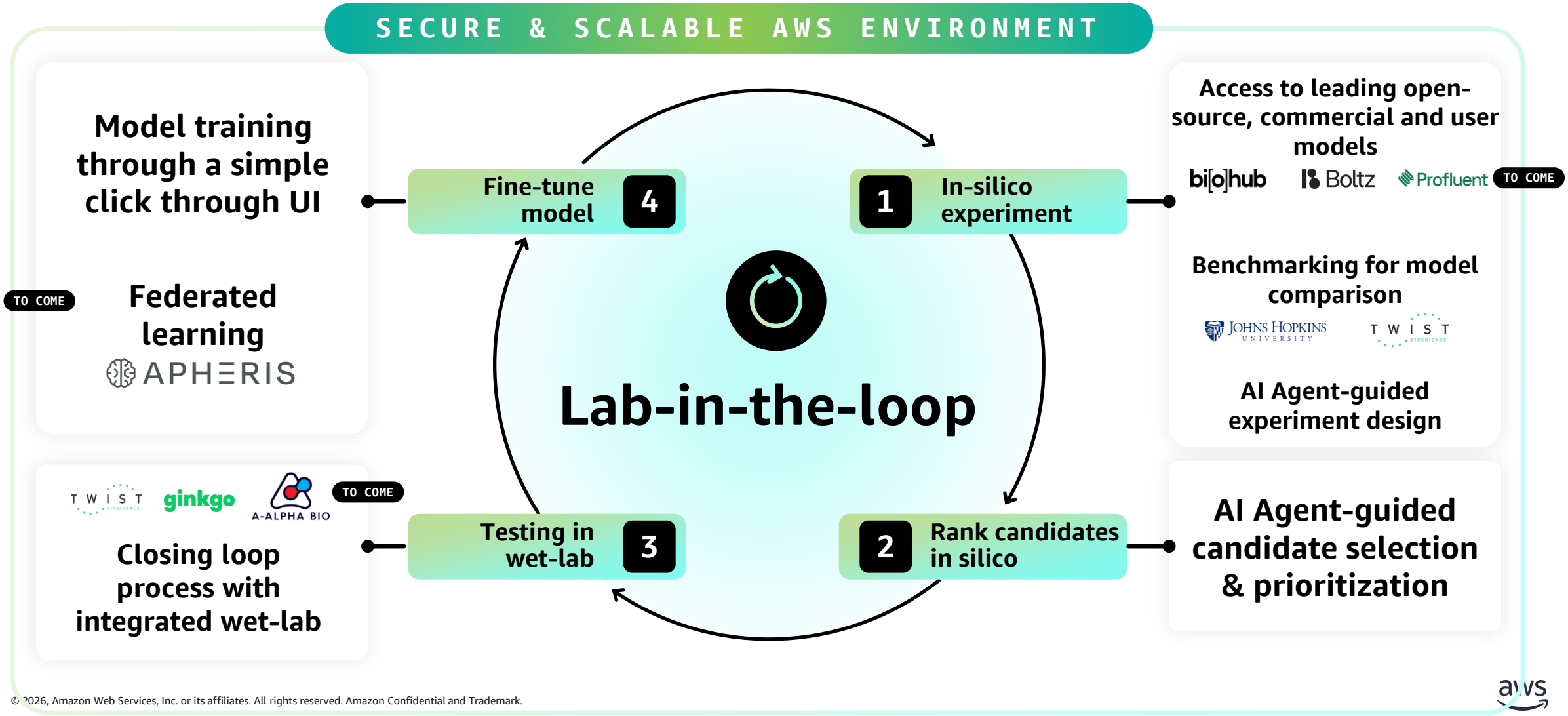
© 2026, Amazon Web Services, Inc. or its affiliates. All rights reserved. Amazon Confidential and Trademark.

Common pain points in performing Lab-in-the-Loop



© 2026, Amazon Web Services, Inc. or its affiliates. All rights reserved. Amazon Confidential and Trademark.

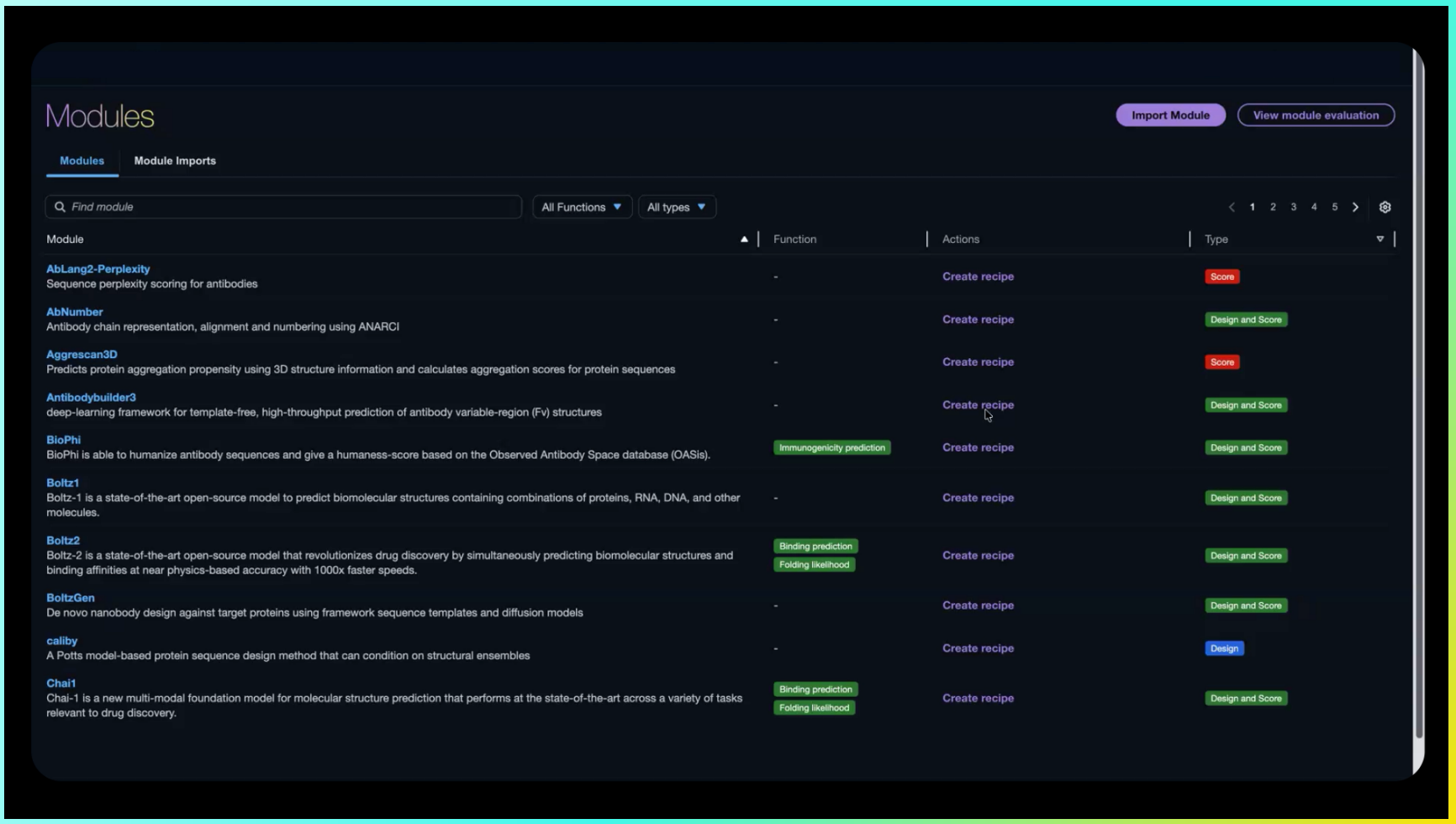
Amazon Bio Discovery – A unified application for AI drug discovery



© 2026, Amazon Web Services, Inc. or its affiliates. All rights reserved. Amazon Confidential and Trademark.

Step 1:
Evaluate and build a custom workflow

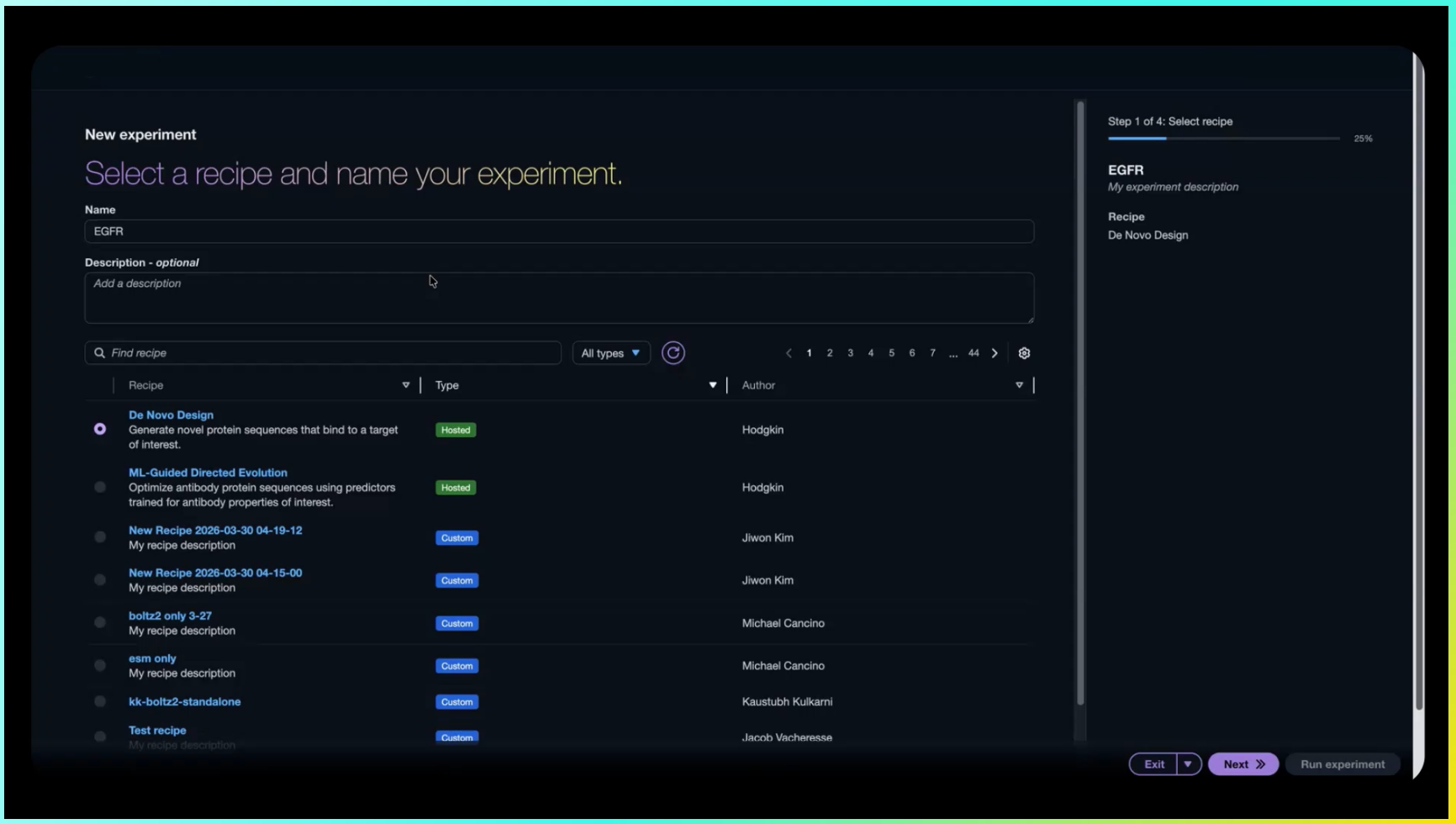
1 2 3 4 5



© 2026, Amazon Web Services, Inc. or its affiliates. All rights reserved. Amazon Confidential and Trademark.

Step 2:
Design an experiment with AI agents

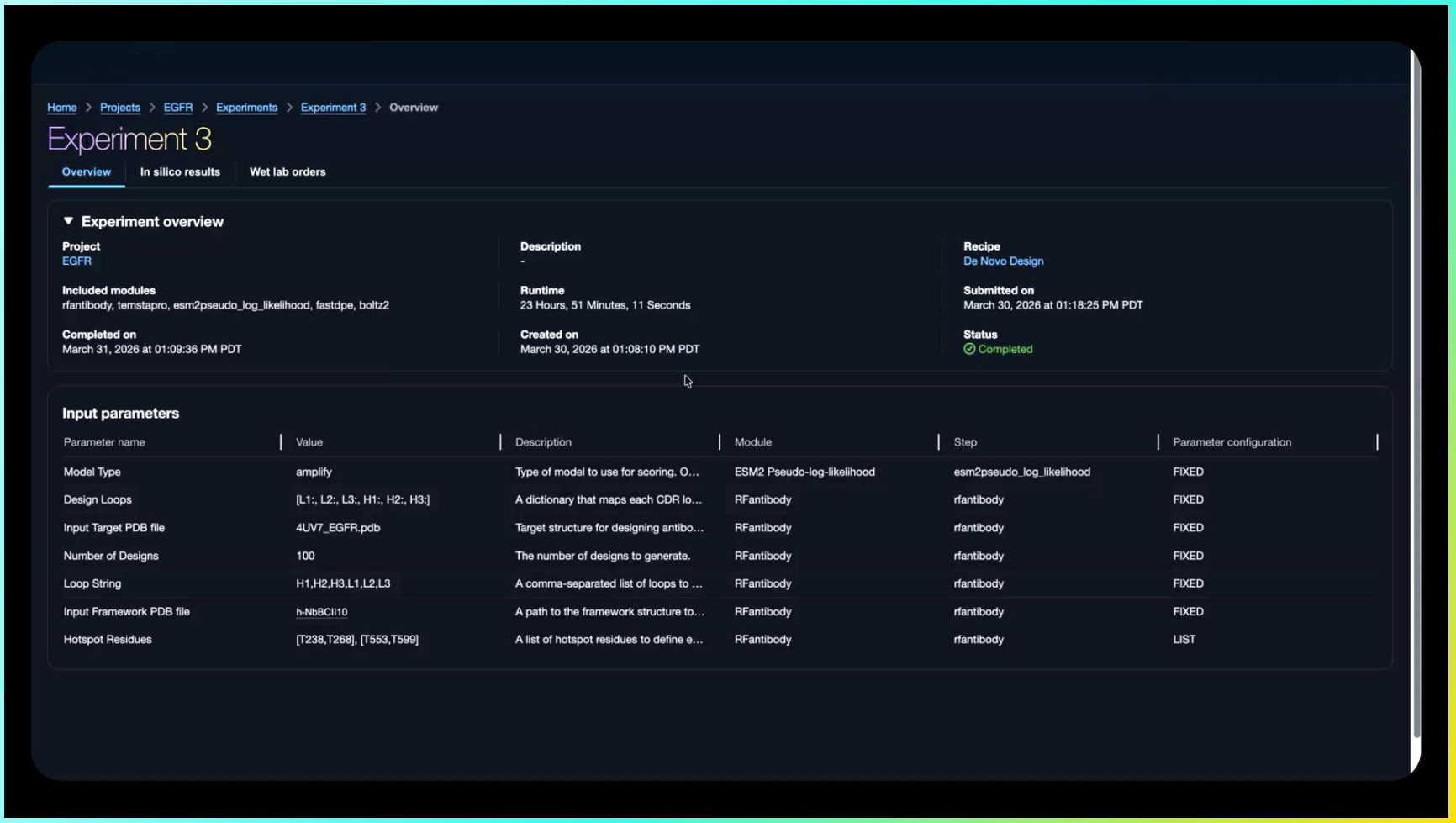
1 2 3 4 5



© 2026, Amazon Web Services, Inc. or its affiliates. All rights reserved. Amazon Confidential and Trademark.

Step 3:
Analyze in silico results and identify the best candidates with agentic assistance

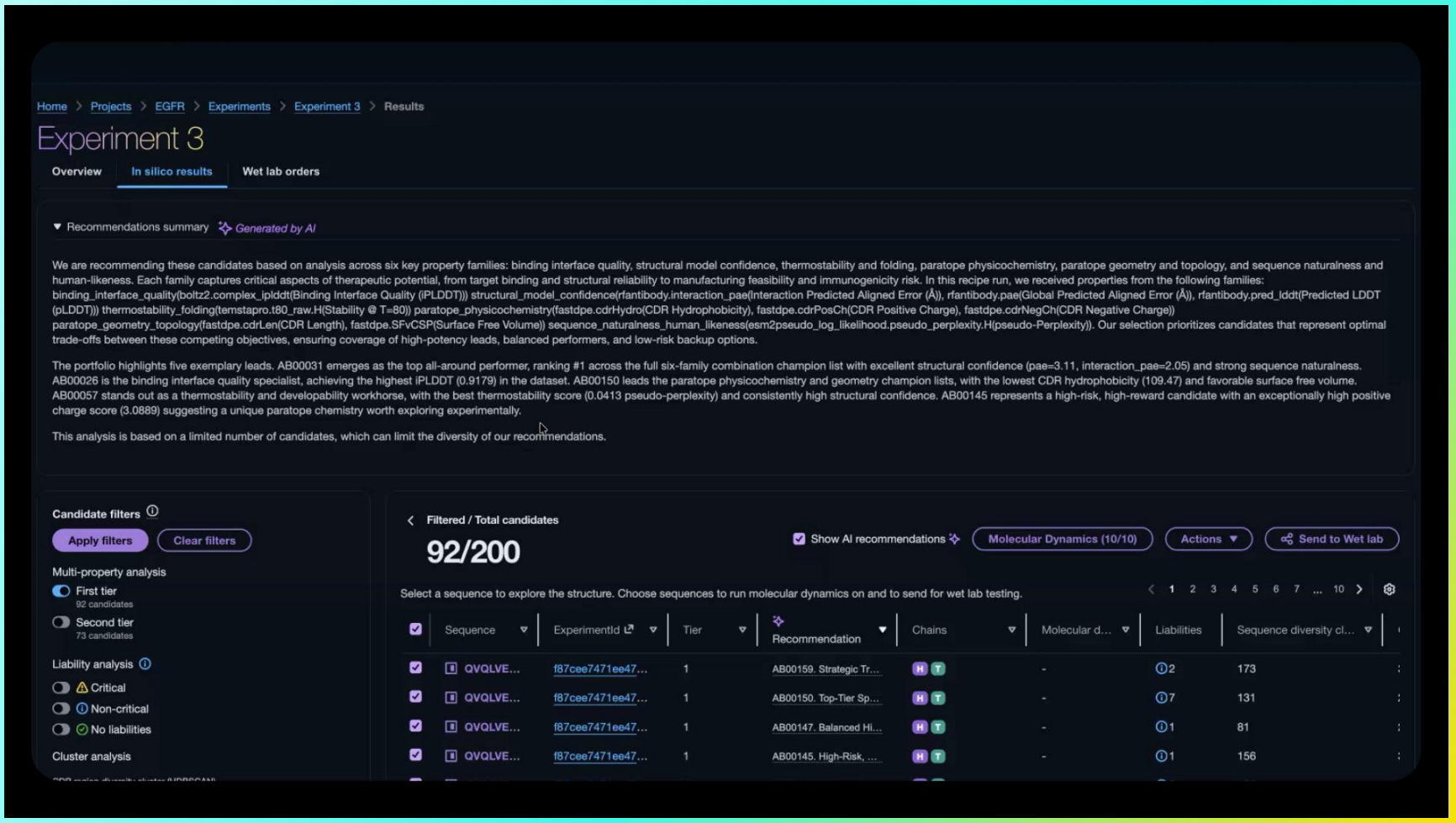
1 2 3 4 5



© 2026, Amazon Web Services, Inc. or its affiliates. All rights reserved. Amazon Confidential and Trademark.

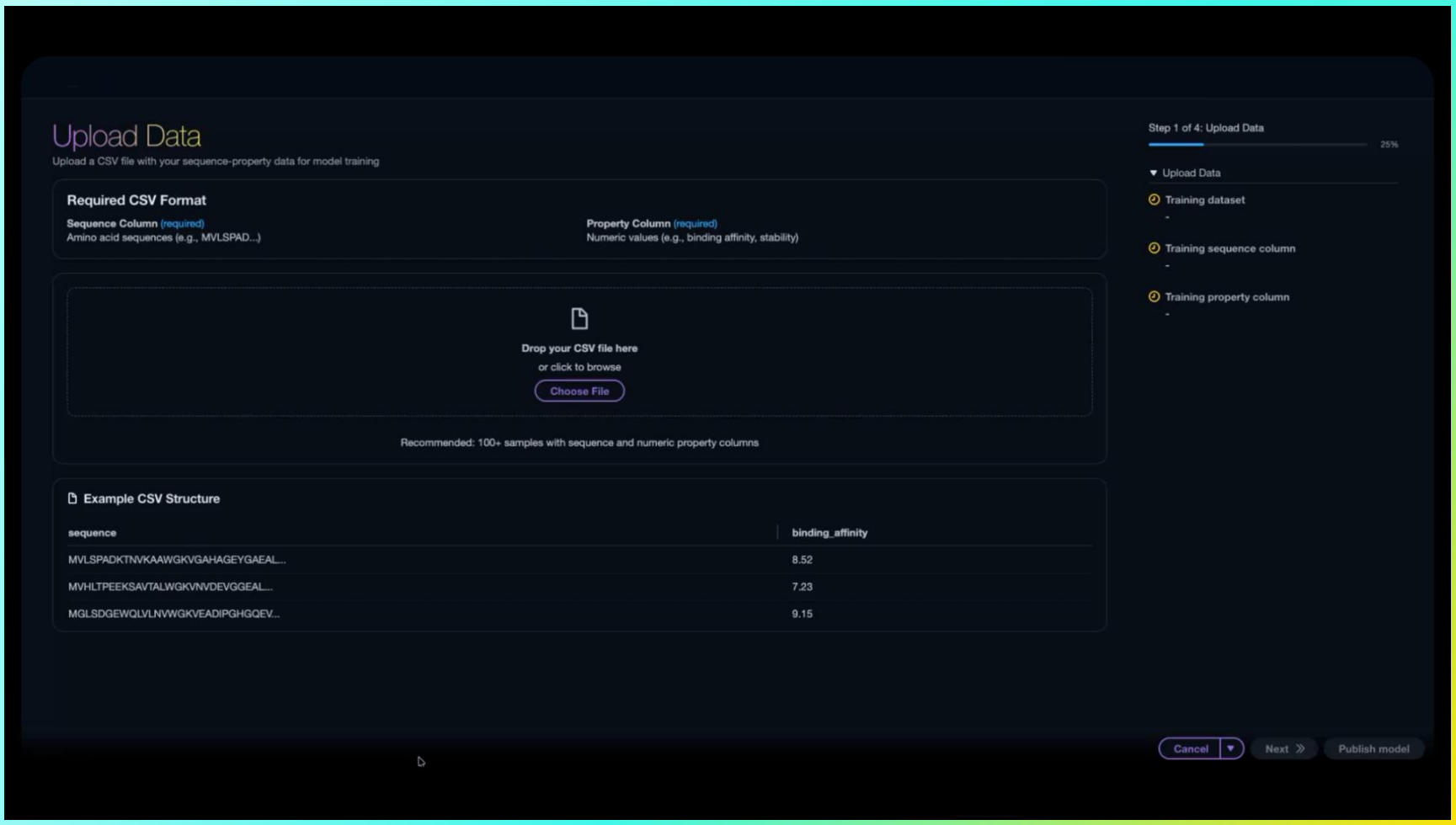
Step 4:
Send to the wet-lab

1 2 3 4 5

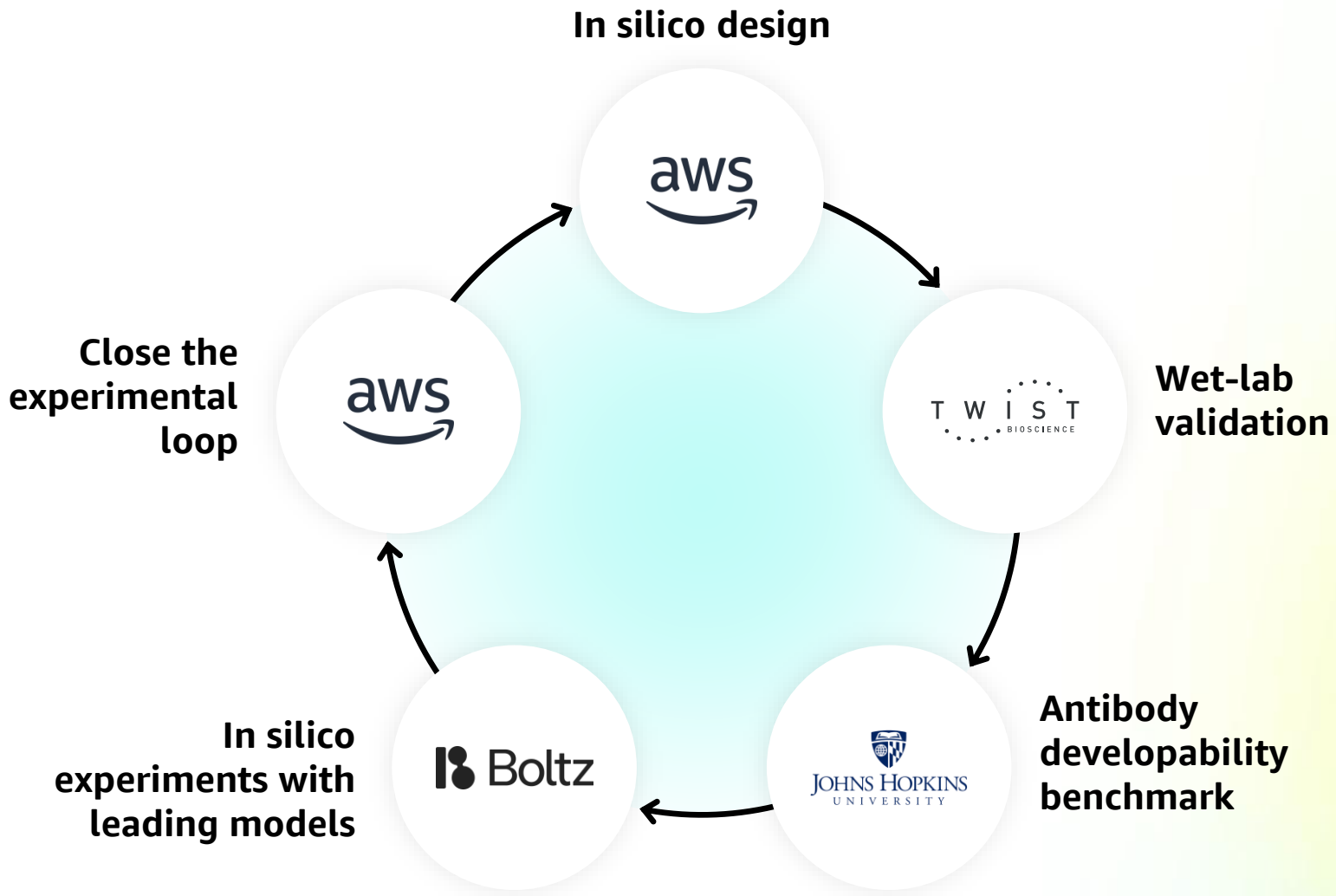


© 2026, Amazon Web Services, Inc. or its affiliates. All rights reserved. Amazon Confidential and Trademark.

Step 5:
Closing the loop by training models with wet-lab data



© 2026, Amazon Web Services, Inc. or its affiliates. All rights reserved. Amazon Confidential and Trademark.



MSK Case Study

REPORT AND RESULTS

Memorial Sloan Kettering Cancer Center

Sub-nanomolar binders (0.66nM to 305nM) found without experimental structure or prior antibody data for a novel Desmoplastic Small Round Cell Tumor target using our AI agents.

© 2026, Amazon Web Services, Inc. or its affiliates. All rights reserved. Amazon Confidential and Trademark.

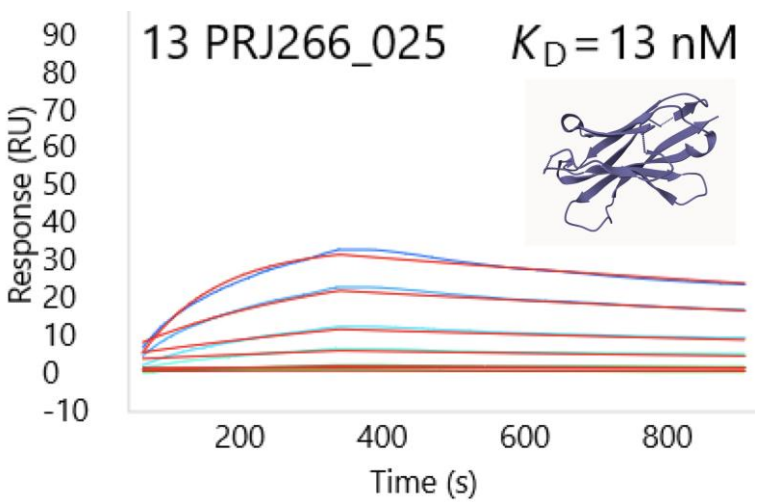
De novo study—validation results

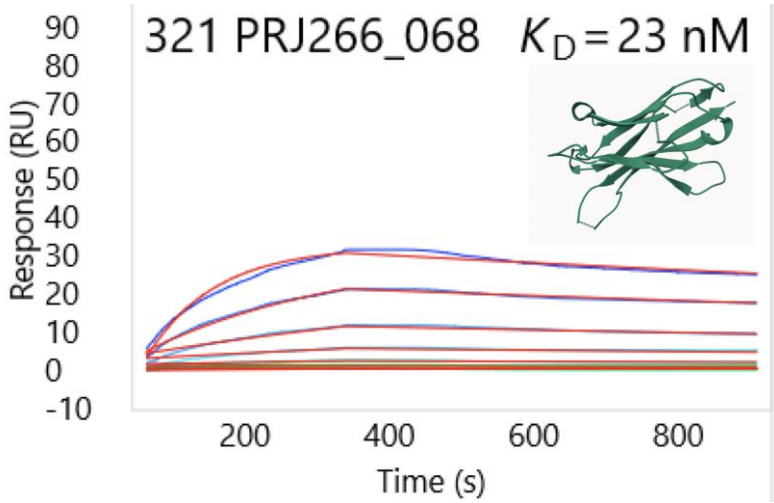
46 out of 116
Candidates tested showed measurable binding affinity

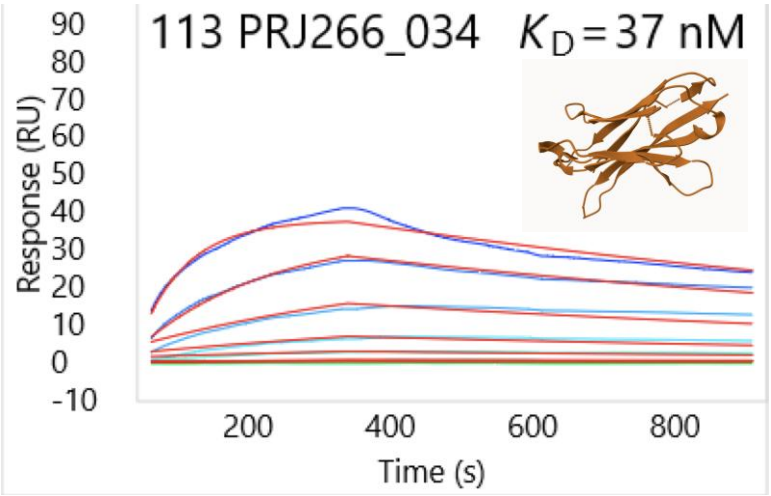
Binders detected across
nM
affinity range

~500
Individual clones selected experimentally

288,000
Sequences designed in silico

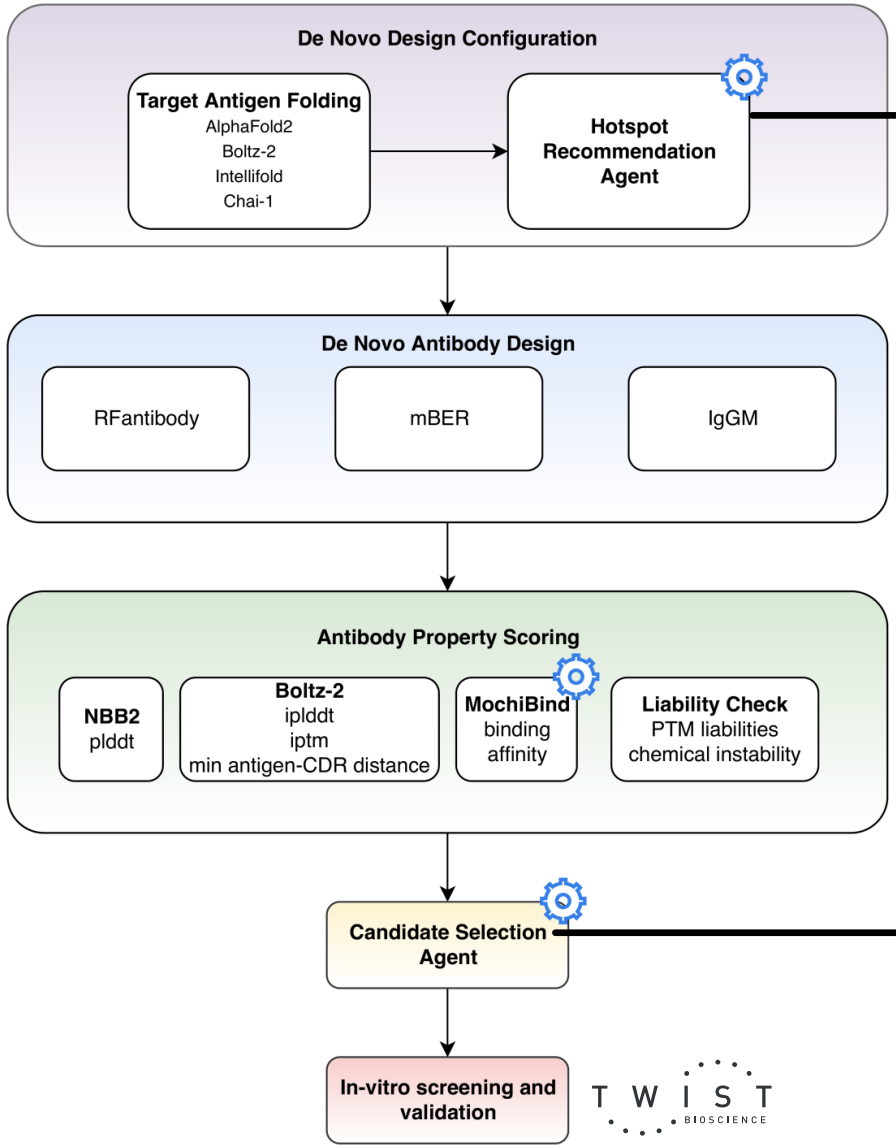


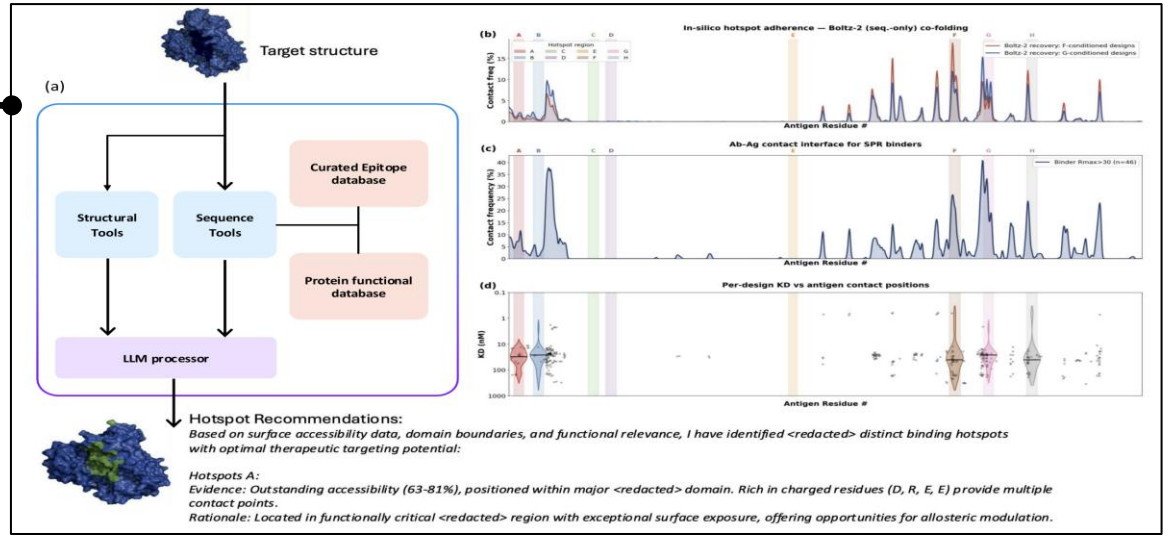


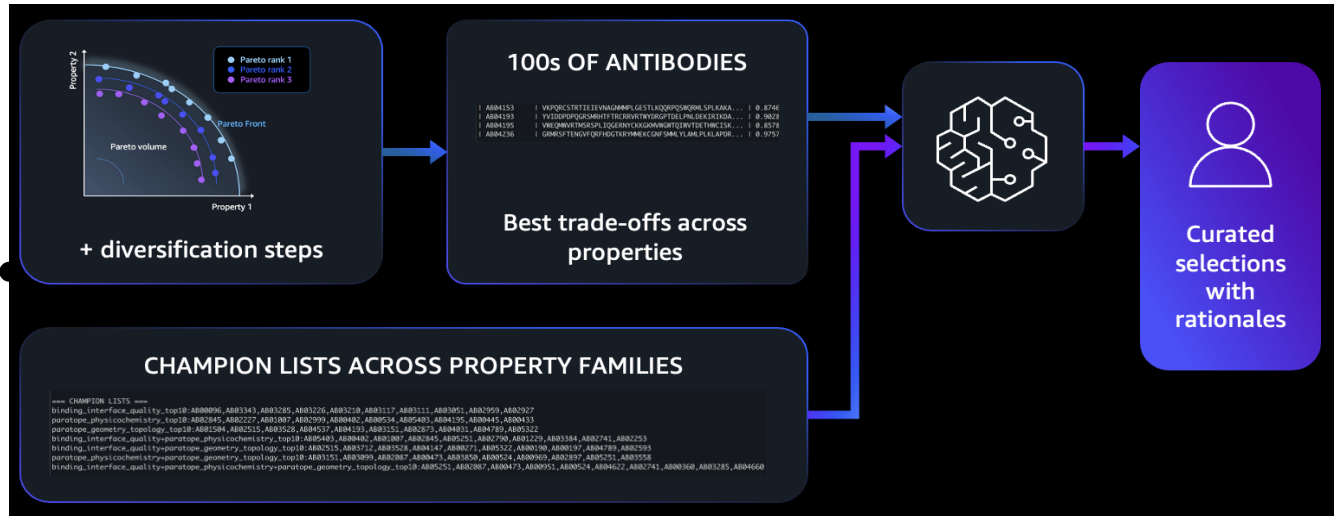


© 2026, Amazon Web Services, Inc. or its affiliates. All rights reserved. Amazon Confidential and Trademark.

De novo design pipeline overview







Internally developed components

Get started!

Free academic tier for users with verified **.edu** or **.org** accounts

Free 30-day trial for all new users

© 2026, Amazon Web Services, Inc. or its affiliates. All rights reserved. Amazon Confidential and Trademark.