FUJIFILM
Value from Innovation

Partners for *Life*

drug2drugs®

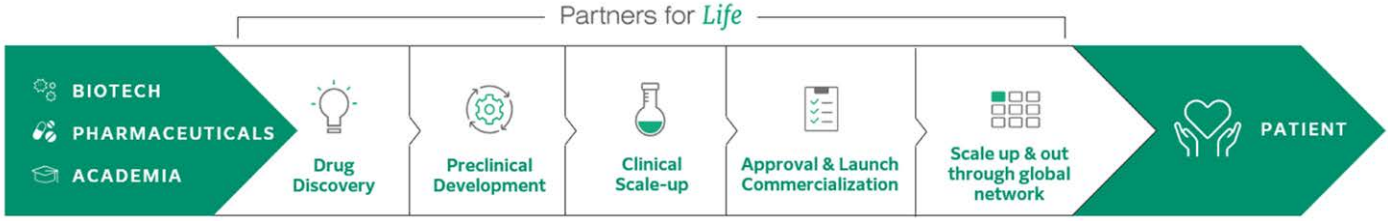
AI-AAM

AI and chemical simulation-based drug discovery support service

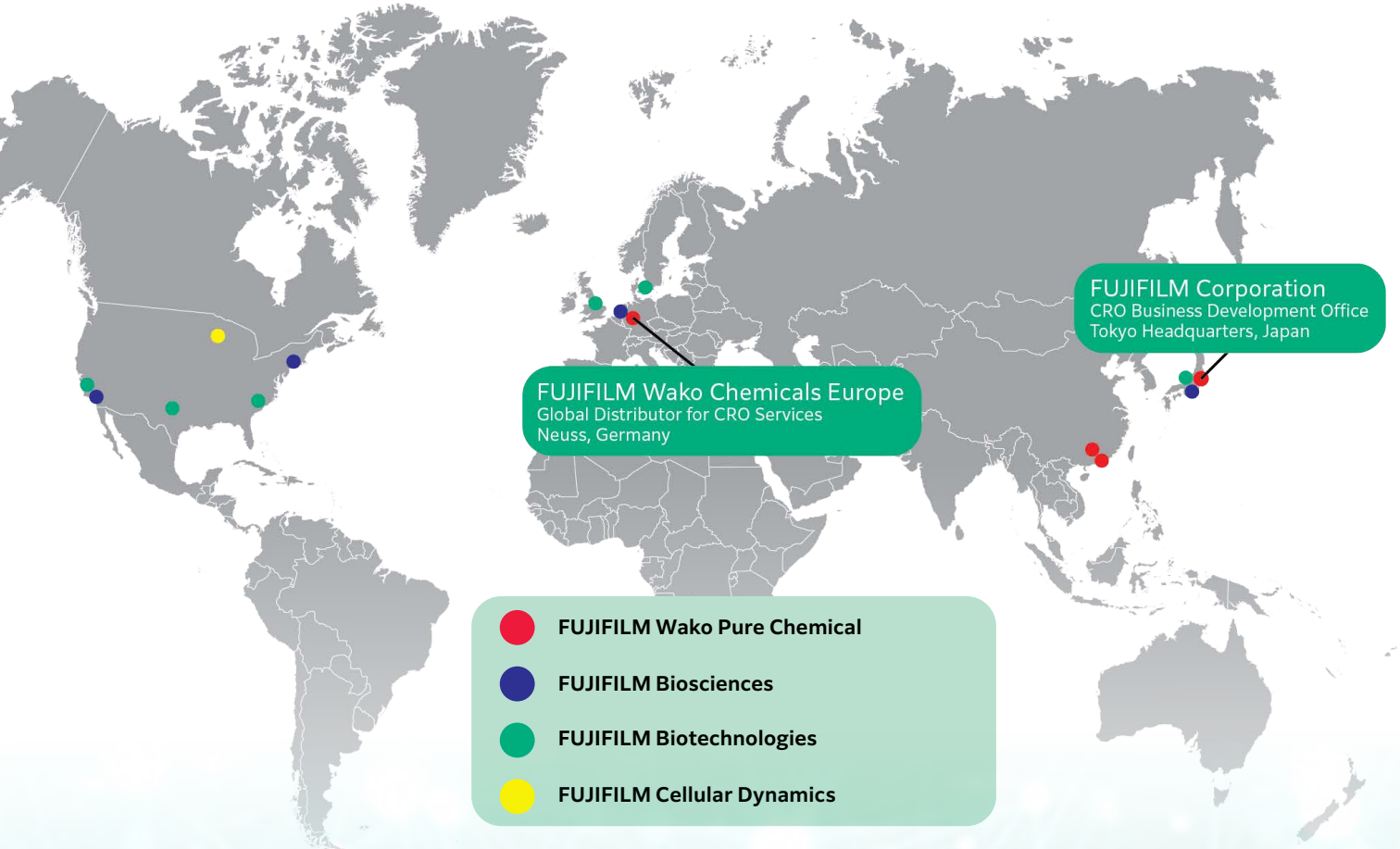
About Us

Partners for *Life*

Fujifilm Life Sciences provides an integrated suite of products, services and solutions backed with deep expertise and a history of innovation to rapidly progress your product to market.



FUJIFILM Wako Pure Chemical is acting as a global distributor for this Japan-based service. We are a general life science company from Japan with almost 100 years of history. Based on advanced technological development, we provide highly functional and high-quality laboratory chemicals, specialty chemicals, and clinical diagnostic reagents as our products, With our presence in Japan and our local subsidiaries globally, we strive to contribute to the life science and chemical industry worldwide.



Our CRO Services

- Based on solid data and innovative research
- Experienced scientists and premium customer service
- Highly customizable service based on customers' needs

View Online

Accelerate Drug Discovery
No Target Required.

drug2drugs AI-AAM® is an AI and chemical simulation-based drug discovery support service which generates many candidate compounds with different scaffolds from the structural information of one active compound. By leveraging our proprietary AI-AAM (amino acid mapping) method, our platform can utilize *de novo* design or library search methods to explore vast chemical space to identify structurally diverse and thermal stable compounds, while also taking care to avoid generating only compounds that are difficult to synthesize. Within just one month turnaround time, drug2drugs AI-AAM® can deliver around 100 candidate compounds that could potentially unlock improved bioactivity, potency, reduced toxicity, IP clearance, or even unlock the possibilities for overhauling the drug delivery mechanism of the drug.

All results are delivered securely and confidentially, accelerating your small molecule and peptide discovery efforts without compromising quality.

Built for Medicinal Chemists. Trusted by Innovators.

ATOM-BASED COMPOUND GENERATION
AI-AAM makes diverse scaffolds, filtering for thermally stable structures.

STREAMLINED LEAD OPTIMIZATION
No target information required. Only 1 month turnaround for computation.

DE-RISK LEAD OPTIMIZATION
Identify better binders, faster.

CONFIDENTIAL & SECURE
Minimal experimental data required. Your IP stays yours.

Top Use Cases

- Changing the core structure to enhance potency
- Finding a candidate compound that avoids structure-derived toxicity
- Generating hits from medium-sized molecules, proteins, and natural compounds to initiate discovery
- Exploring backup compounds
- Identifying IP-cleared scaffolds

Why choose drug2drugs AI-AAM®?

1 **Save Time and Costs in R&D**
ROI for drug discovery efforts has been falling industry-wide. Innovate smarter with **drug2drugs AI-AAM®.**

2 **Explore Novel Scaffolds**
Increase your chances of discovering a successful drug candidate or improving aspects of an existing drug.

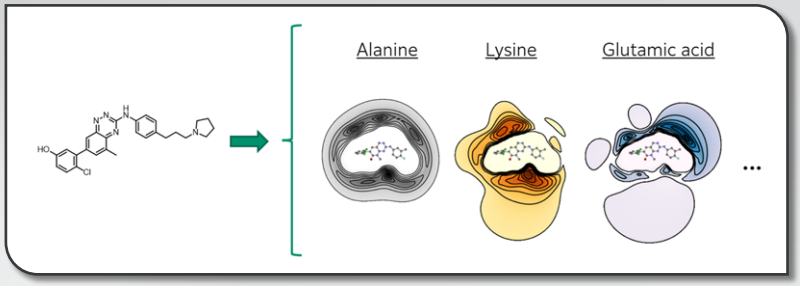
3 **No Need for Large Data**
Only the structural information of the bioactive region of your compound is required.

4 **IP-Clean Backup Compounds**
Rapidly generate patent-safe analogs to safeguard your lead series or navigate IP constraints.

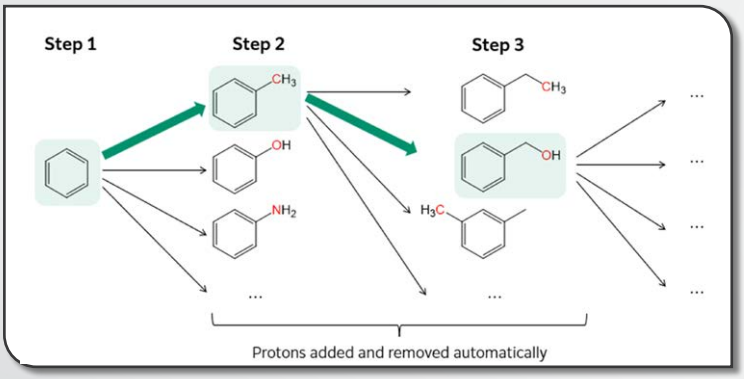
How AI-AAM Reimagines Your Chemistry

AAM descriptors enable fast and accurate prediction of bioactivity

Unlike traditional methods that require detailed 3D protein structures and lengthy binding energy calculations, our **AI-AAM method** compares compounds by measuring the similarity between their AAM descriptors, which are essentially their "pseudo binding sites" generated directly from the compounds themselves. If two compounds have similar AAM patterns, they are predicted to bind with comparable strength, allowing us to quickly identify promising drug candidates without needing complex protein data. This makes our predictions not only accurate, but also at least 10,000 times faster than quantum mechanical methods, revolutionizing the speed of drug discovery.

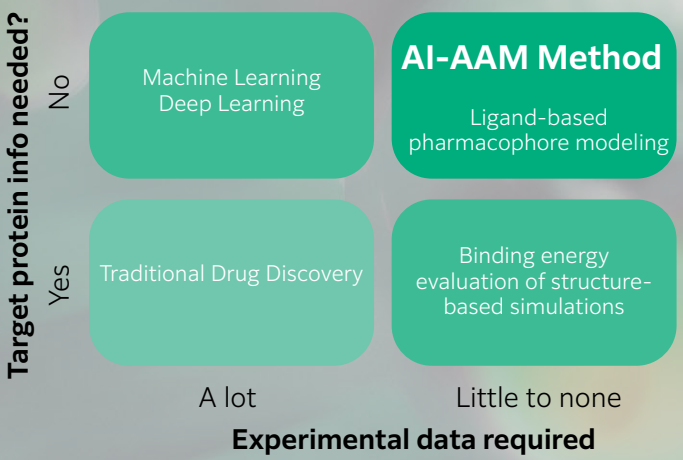


Unique structural design AI for diverse structure generation



Our proprietary AI compound structure generator creates novel drug candidates by building molecules atom by atom, starting from scratch and evolving compounds with high similarity to the target's AAM descriptor. Unlike traditional fragment-based methods, which swap parts of known molecules and often produce limited structural diversity, our atom-by-atom design explores an immense chemical space of up to 10^{60} possibilities. To ensure practical application, our AI incorporates a thermal stability index derived from analyzing over 100 million compounds, filtering out unstable designs early. By progressively adding atoms and selecting candidates based on AAM similarity and stability, our system produces structurally diverse compounds that maintain desired bioactivity profiles. Our approach accelerates drug discovery by delivering a broad variety of promising candidates that traditional methods cannot match.

What Makes AI-AAM Different



- **Orders of magnitude faster.** AAM similarity is computed in seconds per compound, ≥10,000x faster than QM/MM contexts.
- **No target structure or sequence required.** Start from a single active compound.
- **Minimal data sharing, strong confidentiality.** Keep biological data in-house.

Service Flow & Deliverables

1 Discussion

Introduction of service, technical team, and initial alignment on price and general project points, facilitated by global business development representatives at FUJIFILM Wako Chemicals Europe (WKEU).

2 Contracts

Conclusion of confidential disclosure agreement (CDA) and master service agreement (MSA) between stakeholder parties via DocuSign. Further technical discussion about project details after signing of CDA.

3 Start of Service

After receiving the structural information about the bioactive region of your key compound, we first perform the conformational calculations to validate our starting point. Then, we compute the AAM descriptors.

4 Library Search

Search our library of 10^8 real compounds to find commercial chemicals with similar AAM to that of the original compound.

4 *De Novo* Design

Design completely new compounds atom-by-atom using our proprietary AI structure generator.

5 End of Service

Deliverables (listed below) are sent confidentially to you by SecureDeliver, invoicing is carried out. Final meeting to discuss the results and next steps for your drug development process.

CUSTOMER

Structural information of the bioactive region of the compound

Deliverables

- Chemical structure and AAM similarity list of the candidate compounds (approx. 100)
- 3D images of the relationship between chemical group and AAM similarity
- Customer support with understanding the details of scaffold transformation for SAR

	AAM Similarity Profiling Service	drug2drugs AI-AAM® Full Service
Service Positioning	Entry module for R&D prioritization	Full solution
Input Required	Compound library or analog series	1 structure, bioactive region of cmpd
Deliverables/ Output	AAM similarity calculations only	3D structures & AAM similarity of candidates

AAM Similarity Profiling Service

A streamlined, lower-cost version of our full drug2drugs AI-AAM® service, this module focuses on computing AAM similarity values for your internal compound library. Ideal for early-stage discovery and SAR exploration, it enables you to quantitatively evaluate structure-activity relationships, identify features that drive selectivity, and select and validate compounds before proceeding to library search and structure generation. Whether you're validating targets, optimizing library design, or clarifying SAR trends, this service helps guide better decisions in drug discovery.

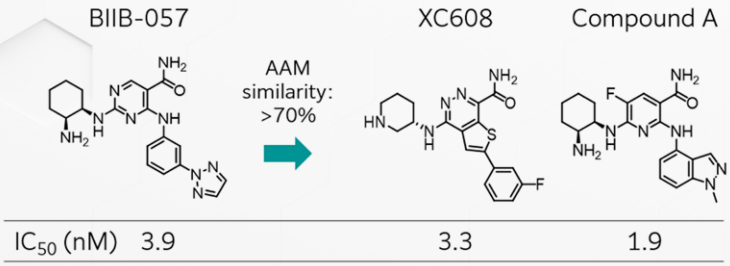
Proof in Practice:
What Our Platform Has Delivered

Case Study 1: Scaffold Hopping (Kinase: Syk)

Goal: Replace the core structure of a known Syk kinase inhibitor (BIIB-057) with a new scaffold, while retaining biological activity.

Process: We analyzed BIIB-057's interaction profile and screened 12 million commercially available compounds for high AAM similarity.

Result: Two new compounds (XC608 and Compound A) with distinct scaffolds were identified. Both showed equivalent or better enzyme inhibition compared to BIIB-057.



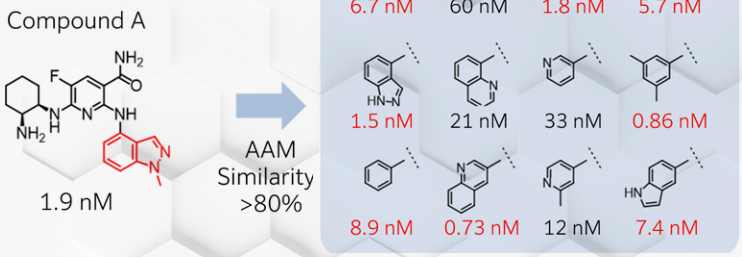
Takeaway: drug2drugs AI-AAM® enables successful scaffold hopping to generate patent-safe compounds with preserved potency, within just one month.

Case Study 2: Lead Optimization

Goal: Improve binding affinity of a lead compound through targeted molecular modifications.

Process: The AI-AAM® method generated 150 analogs with >80% AAM similarity. 12 were selected and synthesized for activity testing.

Result: IC_{50} values ranged from 0.73 to 60 nM, and several had much stronger affinity than the original lead.



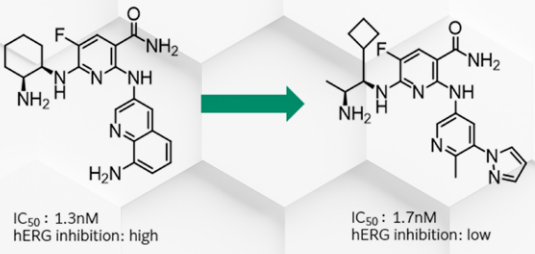
Takeaway: AI-AAM accelerates SAR optimization by delivering potent, synthesizable candidates, streamlining the design-make-test cycle.

Case Study 3: Reducing Toxicity While Maintaining Potency

Goal: Eliminate hERG inhibition from a potent SYK inhibitor to improve cardiac safety, without compromising efficacy.

Process: Combined our AI-AAM® de novo design capabilities with a ML-based hERG predictor to redesign a lead compound (IC_{50} = 1.3 nM) known to inhibit hERG.

Result: Identified and synthesized a new analog with low hERG inhibition and similar potency (IC_{50} = 1.7 nM).



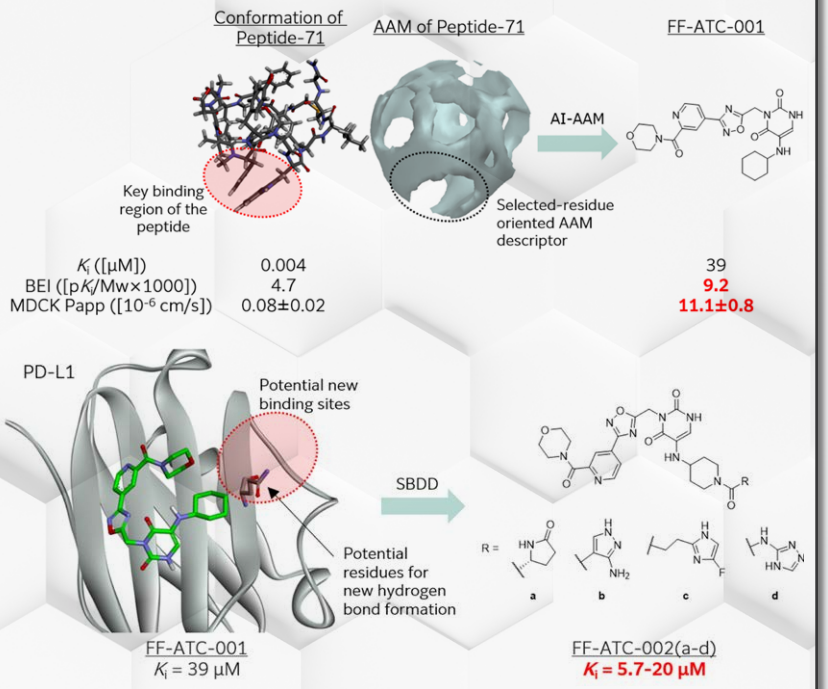
Takeaway: drug2drugs AI-AAM® enables safety-focused lead optimization, maintaining efficacy while minimizing toxicity risks.

Case Study 4: Peptide-to-Small Molecule Conversion (PD-L1)

Goal: Convert a macrocyclic peptide into small-molecule compounds that efficiently bind to PD-L1.

Process: We applied our novel AI-AAM strategy to generate small-molecule candidates from the peptide and further optimized their activity using structure-based design.

Result: We successfully obtained bioactive small-molecule compounds from the macrocyclic peptide by leveraging detailed binding information of the peptide with the AI-AAM strategy. Furthermore, structure-based drug design (SBDD) enabled us to generate multiple hit compounds with enhanced activity.



Takeaway: AI-AAM® can transform intracellular-inaccessible peptides into drug-like small molecules, unlocking the potential for oral delivery of traditionally injectable modalities.

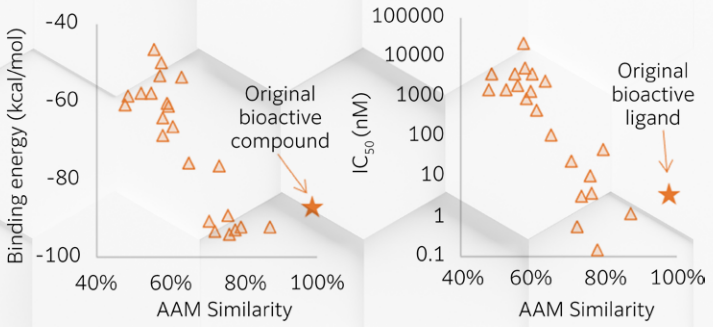
Case Study 5: AAM Similarity Analysis (Kinase Syk)

Goal: Find compounds with similar binding affinity without protein structures using AAM.

Process: Selected compounds by AAM similarity; checked binding energy and bioactivity.

Result: AAM matched binding affinity to the original ligand.

Takeaway: AAM enables analysis of the relationship between molecular structure and activity, even without protein structural information.



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Scan the QR code and send us an inquiry to schedule a meeting and get started!

dge-CRO-inq@fujifilm.com

Available to customers globally.

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Contact Us

For any inquiries, please send us an email at:
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