

A RaaS platform that supports research as a service.

Amaterus AI is a RaaS (Research as a Service) platform that integrates chemistry AI to support R&D and decision-making. It connects knowledge and database creation, synthesis route exploration, reaction prediction and validation, and conceptual process design to guide how to make it.

Research as a Service

Access the knowledge, AI, and calculations needed for research as a service, with knowledge creation, exploration, validation, and conceptual design connected in one platform. Apply the insights to your next experiments and candidate selection to support R&D and decision-making.

Shorten development time

Connect knowledge organization, route exploration, reaction validation, and conceptual process design to advance R&D.

Reduce R&D costs

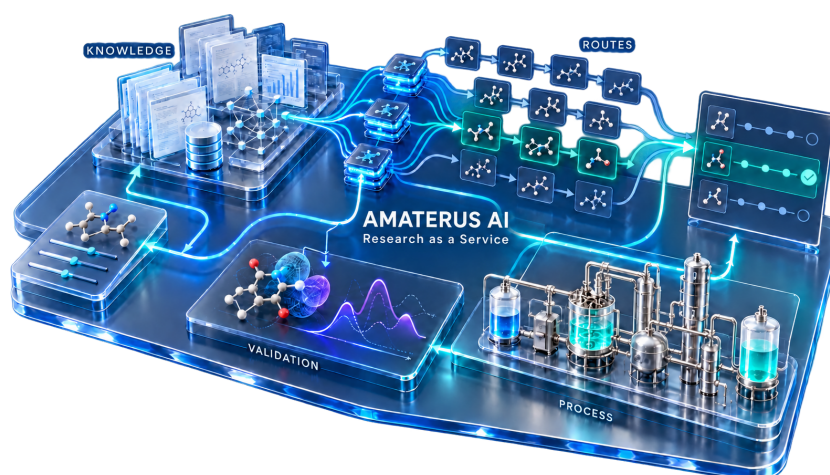
Use accumulated knowledge and advance validation to reduce duplicated experiments and investigations.

Improve decision quality

Evaluate diverse candidates using data and calculations to make evidence-based decisions.

Focus research resources on promising candidates

Select promising synthesis routes and focus experiments, people, and computing resources on them.



Chemistry AI that connects your R&D workflow.

Turn internal experimental data, papers, and patents into usable knowledge. Select promising synthesis routes from diverse candidates, check reaction feasibility, and develop a process concept covering steps and reaction conditions.

Knowledge & database creation AI

Convert internal experimental data, papers, patents, and other sources into organized knowledge that can be put to use.

Synthesis route exploration AI

Multiple route exploration AIs generate diverse candidates, and consensus AI selects promising synthesis routes.

Reaction prediction & validation AI

Check reaction feasibility in advance using data and quantum chemistry calculations.

Conceptual process design AI

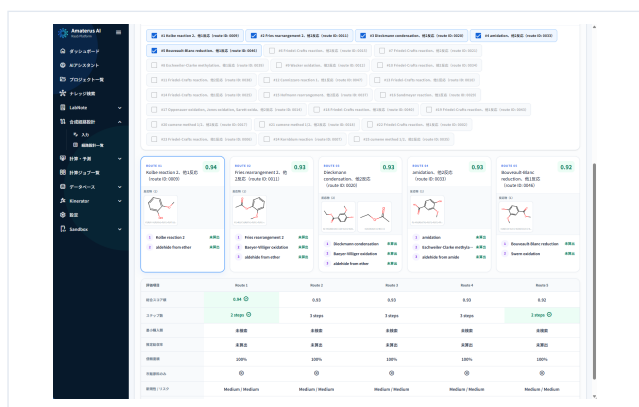
Develop a conceptual process design, including steps and reaction conditions, based on the synthesis route.

Screens from the research workflow

Compare candidates, inspect evidence, work with knowledge, and explore molecular structures in one environment.

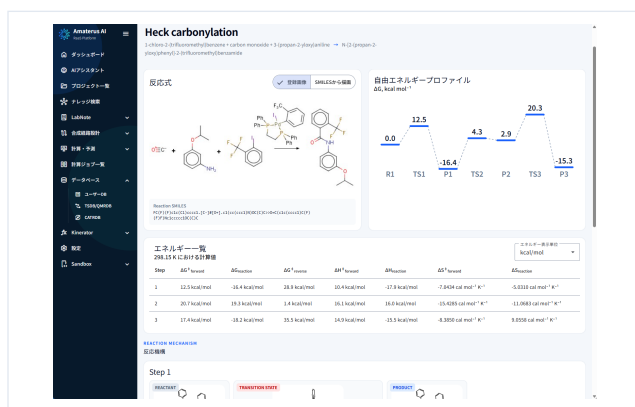
01

Compare candidate routes side by side



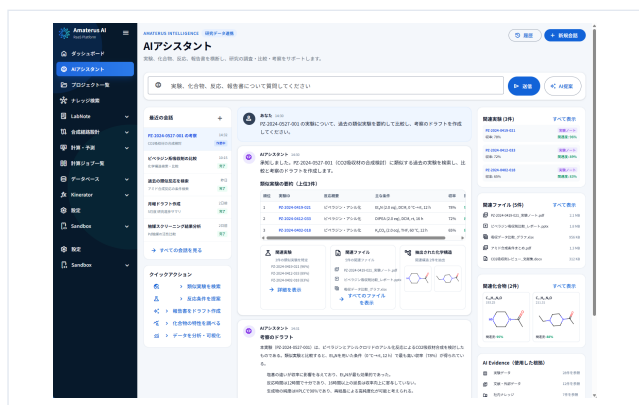
02

Reaction evaluation database: reactions and calculation evidence



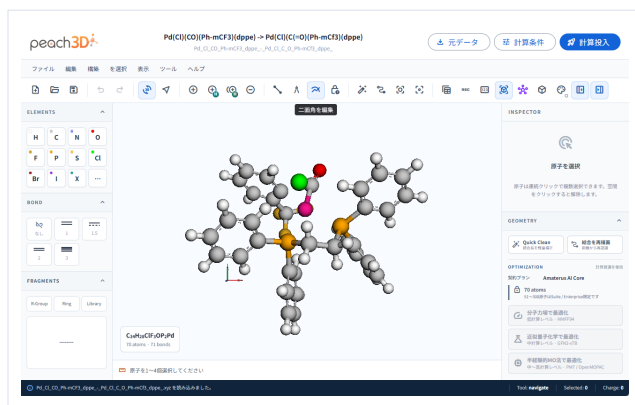
03

AI assistant: review information across experiments and documents



04

peach3D: inspect structures and prepare calculations



Screens illustrate the workflow. Displayed scores do not guarantee experimental success or yield.

[View product screens on the website](#)

For the people who conduct and support R&D.

Synthetic & process chemists

Compare alternatives to existing routes or paths from available starting materials. Narrow candidates while checking reaction evidence and the steps that need further validation.

Research managers

Review route decisions, their reasons, unresolved questions, and the next experiments or calculations without rebuilding the project context for every progress review.

R&D DX & information teams

Connect documents and experimental information to structures, reactions, and conditions. Preserve sources and support knowledge reuse across research themes.

IT, security & governance

Review data location, permissions, identity, logging, retention, deletion, and integration alongside the usability needs of research teams.

From knowledge to your next R&D task.

Turn internal experimental data, papers, and patents into usable knowledge. Select promising synthesis routes from diverse candidates, check reaction feasibility, and develop a process concept covering steps and reaction conditions.

Use knowledge to develop a path to how to make it.

Knowledge & database creation AI → Synthesis route exploration AI → Reaction prediction & validation AI → Conceptual process design AI

1. Knowledge & database creation AI

Convert internal experimental data, papers, patents, and other sources into organized knowledge that can be put to use.

2. Synthesis route exploration AI

Multiple route exploration AIs generate diverse candidates, and consensus AI selects promising synthesis routes.

3. Reaction prediction & validation AI

Check reaction feasibility in advance using data and quantum chemistry calculations.

4. Conceptual process design AI

Develop a conceptual process design, including steps and reaction conditions, based on the synthesis route.

Inform the next R&D task

Review the exploration, validation, and conceptual design results as a research team and use them to plan the next experiments and investigations. Organize new experimental data as knowledge for subsequent R&D.

Prepare a focused evaluation

Choose a task and use your current workflow as the baseline. Review relevant capabilities and data storage in a demonstration, then agree on the evaluation scope and how results will be reviewed.

Plans & pricing

Choose Core for synthesis route design and selection. Extend to Suite for proprietary knowledge, reaction evaluation, and process design. For dedicated environments or advanced internal integrations, Enterprise builds on Core or Suite to meet your deployment and operational needs.

Amaterus Core · \$31,000+ per year

About 5 standard users; additional seats available. Standard support and help getting started. Annual organization-level contract. Generate and compare synthesis routes, and record the evidence and decisions behind your selections. Use lab notebooks, up to five user databases, knowledge search, basic quantum chemistry calculations, and project and job management.

Amaterus Suite · \$125,000+ per year

About 20 standard users; additional seats available. Priority support and implementation assistance. Standard price; individual quote based on your requirements. Use advanced route design, knowledge creation, quantum chemistry reaction evaluation, and process design in one environment. Includes basic API and SSO integration. Currently available to a limited number of companies.

Amaterus Enterprise · Custom quote

Designed for your users, departments, and sites. Custom SLA, dedicated assistance, and operational design. Quoted for your required capabilities and configuration. Build on Core or Suite with internal reaction database integration, internal knowledge collection and reuse, and dedicated environments. Tailor system integration, service levels (SLAs), and operations to your requirements.

Getting started with Suite

Suite is currently available to a limited number of companies. Tell us about your research tasks and team size. We will review the data volume, compute resources, integrations, and implementation scope you need and discuss terms and pricing with you.

Planning your Enterprise deployment

Enterprise combines Core or Suite with the features, dedicated environments, and internal integrations you need. We will discuss your preferred configuration and operations, then provide a proposal and quote.

Features & services	Core	Suite	Enterprise
A. Synthesis route design			
Consensus AI retrosynthesis route design	✓	✓	✓
Multiple synthesis route engines and preset knowledge bases	✓	✓	✓
Route trees, rankings, and score comparisons	✓	✓	✓
Reaction condition prediction, commercial availability, and indicative prices	✓ Basic	✓	✓
Route score breakdowns	✓ Basic	✓	✓
Reaction evaluation integration with quantum chemistry calculations	✓ Partial	✓	✓
Forward and hybrid forward/retrosynthesis route design	-	✓	✓
Detailed route engine settings (Advanced Mode)	-	✓	✓
Engine knowledge bases built from your own reaction databases	-	✓	✓
Enterprise reaction database integration and related information	-	-	✓
Edge Knowledge / Crawler for automatic knowledge and database creation	-	-	✓
B. Knowledge and chemical information assets			
Electronic lab notebooks	✓	✓	✓
User database creation and import	✓ Up to 5	✓	✓
Knowledge search	✓	✓	✓
AI assistant	✓ Limited functionality	✓ Included allowance + usage-based	✓ Custom configuration
Hybrid Knowledge Edge for internal chemical information assets	-	-	✓
C. Reaction evaluation (quantum chemistry)			
Quantum chemistry calculations and reaction analysis	✓ Basic	✓	✓
Compute resources	✓ Shared	✓ Dedicated	✓ Custom design

Features & services	Core	Suite	Enterprise
High-accuracy quantum chemistry calculations	-	✓	✓
Quantum chemistry reaction databases (TSDB/QMRDB)	-	✓ Basic	✓
Import of user calculation results	-	✓	✓
Catalytic reaction database (CATRDB)	-	-	✓
D. Conceptual Process Design			
Reaction kinetics simulator (Kinerator)	-	✓	✓
Process optimization	-	✓	✓
Process simulator	-	✓ Basic	✓
E. Organization / Integration / Operations			
User seats	5 / Additional seats available	20 / Additional seats available	Custom design
Project management	✓	✓	✓
Data sharing within the organization	✓	✓	✓
Contract and collaborative research coordination	✓	✓	✓
API / external system integration	Optional	✓ Basic	✓
SSO / identity management / audit	-	✓ Basic	✓
Dedicated database, tenant, and compute environment	-	Optional	✓
ELN / LIMS / internal database / HPC integration	-	Optional	✓
Custom SLA, staged acceptance, and operational design	-	-	✓

✓: Included · Basic / Partial: basic or selected capabilities included · Optional: additional contract · —: not included as standard Enterprise capabilities are configured to your requirements. The scope depends on the Core or Suite capabilities you select and your individual contract. Prices exclude tax. Contracts are organization-based. Costs vary with users beyond the standard seats, compute, storage, data volume, external integrations, dedicated environments, and SLAs. USD reference exchange rate: US\$1 = JPY 160.

Research data & deployment

We do not use your research data to train models without your explicit permission. Your contract defines permitted uses, storage location, retention periods, deletion, export, and confidentiality.

Standard cloud (Core / Suite)

Access a shared cloud managed by TS Technology through your Web browser. The standard deployment for Core and Suite.

Dedicated Cloud / customer VPC (Enterprise)

Deploy applications and databases in a dedicated tenant or your own cloud environment, with data separation and custom service levels (SLAs).

Hybrid Knowledge Edge (Enterprise)

Keep source documents and raw data inside your organization. Share only approved knowledge data, search indexes, and metadata with the cloud.

Internal access with cloud processing (Enterprise)

Connect to approved cloud services through an internal URL or gateway while retaining your internal access point and authentication.

On-premises / private cloud (Enterprise)

Run applications, databases, information collection, and compute in your own environment, supporting isolated networks and fully internal operations.

Define what to evaluate

Define what to evaluate in terms of development time, R&D costs, decision quality, and concentration of research resources on promising candidates. Use the current workflow as the comparison baseline.

Your first conversation

You do not need to send confidential structures or unpublished data in an initial inquiry. Begin with a description of the task.

Explore the product in detail

The website includes dedicated pages for features, screens, the research workflow, getting started, security, and license terms.

Transition State Technology Company Limited

Contact us to discuss a product demonstration or an implementation for your research team.

<https://amaterus.ai/en/contact/>