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COURSE BROCHURE

# AI-Driven Drug Discovery and Development Training Course

28 February – 4 March 2027
Kuala Lumpur

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Registered in the United Kingdom and Saudi Arabia

# AI-Driven Drug Discovery and Development Training Course

**Ref:** 696_26036 **Date:** 28 February – 4 March 2027 **Location:** Kuala Lumpur **Fees:** 4900 GBP

AI-Driven Drug Discovery and Development is a 1-week training course for pharmaceutical R&D managers and clinical development leads, who build an AI Discovery Portfolio Brief setting out where machine learning enters target selection, compound screening and trial design. Discovery cycles are long and attrition is costly, so organisations now ask which predictive models deserve a place in the pipeline and what evidence they need. Jupiter Prime Training runs AI-Driven Drug Discovery and Development for leaders who steer that pipeline.

## Why AI-Driven Drug Discovery and Development Matters Now

Three forces shape the field: protein structure prediction and generative chemistry that open targets once thought undruggable, the growth of omics, imaging and real-world datasets that feed predictive models, and regulators and ethics committees who expect computational evidence to be traceable and reproducible. A research organisation that validates its models carefully shortens design cycles and stops weak candidates earlier; one that trusts unvalidated predictions risks expensive late failures and evidence packages that reviewers reject. The course draws on ISO/IEC 42001 for AI management systems and the NIST AI Risk Management Framework NIST AI RMF to keep scientific models accountable.

## Who Gains Most from AI-Driven Drug Discovery and Development

- Leaders responsible for target validation and early discovery portfolios
- Heads of medicinal chemistry and screening who decide which compounds advance
- Owners of translational and biomarker strategy linking laboratory and clinic
- Clinical development leads who design protocols and choose trial populations
- Research informatics heads who own scientific data and model platforms

Biotech and pharmaceutical R&D units gain most when a discovery scientist, a clinical lead and a data platform owner attend together.

## AI-Driven Drug Discovery and Development Capabilities

Participants learn to judge where a predictive model shortens the path from hypothesis to candidate, and where wet-lab or clinical evidence must still decide.

- Assess target hypotheses ranked by knowledge-graph and omics models — portfolio boards
- Weigh virtual screening hits against assay confirmation costs — medicinal chemistry leads
- Apply predicted protein structures with stated confidence limits — structural biology teams
- Design trial enrichment and site selection using predictive cohorts — clinical development leads
- Specify model validation and data lineage records — quality and regulatory affairs

- Communicate model uncertainty to scientific review committees — R&D leadership

## Key AI-Driven Drug Discovery and Development Terms

- Target identification — finding a protein or pathway whose modulation is likely to change the course of a disease.
- Virtual screening — ranking large compound libraries by predicted binding or activity before any laboratory testing.
- Protein structure prediction — computing a protein's three-dimensional shape from its amino acid sequence, with per-region confidence scores.
- ADMET prediction — estimating absorption, distribution, metabolism, excretion and toxicity of a compound from its structure.
- Trial enrichment — selecting participants most likely to show a measurable treatment effect, reducing sample size and duration.
- Model applicability domain — the chemical or biological space in which a model's predictions remain reliable.

## AI-Driven Drug Discovery and Development Day by Day

### Day 1: The Computational Discovery Landscape

- Pipeline Attrition Mapping — Where Prediction Saves Time and Cost
- Scientific Data Assets Inventory — Omics, Assay and Imaging Readiness
- FAIR Data Principles — Reusability of Laboratory Records
- NIST AI RMF Map Function — Risks of Scientific Models
- Build, Partner or License Choices — Computational Platform Strategy

### Day 2: Targets and Structures

- Knowledge Graph Target Ranking — Prioritising Disease Hypotheses
- Genetic Evidence Scoring — Confidence in Target Validity
- Predicted Protein Structures — Using Confidence Scores Responsibly
- Binding Pocket Detection — Druggability Calls for New Targets
- Target Product Profile Drafting — Linking Biology to Clinical Need

### Day 3: Molecules and Screening

- Virtual Screening Workflows — Narrowing Libraries Before Assays
- Generative Chemistry Models — Proposing Novel Scaffolds
- ADMET Prediction — Early Removal of Unsafe Candidates
- Active Learning Cycles — Choosing the Next Compounds to Synthesise
- Applicability Domain Checks — When Predictions Stop Being Trustworthy

### Day 4: Clinical Development and Evidence

- Predictive Cohort Selection — Trial Enrichment and Inclusion Criteria
- Site Feasibility Models — Recruitment Speed Across Locations
- Synthetic Control Arms — Limits of External Comparator Data
- Model Validation Dossiers — Evidence Reviewers Expect to See
- Data Lineage and Audit Records — Reproducibility of Computational Results

## Day 5: Practising the AI Discovery Portfolio Brief

- Oncology Target Case — Applying Knowledge Graphs and Structure Prediction
- Rare Disease Trial Case — Applying Predictive Cohorts and Enrichment
- Screening Cascade Redesign — Applying Virtual Screening and ADMET Models
- ISO/IEC 42001 Controls for Research Models — Owners and Escalation
- AI Discovery Portfolio Brief — Models, Evidence, Gates and Owners

## Applying AI-Driven Drug Discovery and Development After the Course

- Run a retrospective test of one virtual screening model against past assay results to define its applicability domain.
- Draft a model validation dossier template for the next trial that uses predictive cohort selection.

## AI-Driven Drug Discovery and Development Questions FAQ

### What is AI-driven drug discovery and development and why does it matter now?

It is the use of machine learning across target selection, compound design, screening and trial planning. It matters now because structure prediction and generative chemistry have matured, while reviewers expect computational evidence to be validated and reproducible.

### Which roles gain most from AI-driven drug discovery and development?

Discovery portfolio leaders, medicinal chemistry heads, translational leads, clinical development leads and research informatics owners gain most. They decide which predictions advance a candidate and which still need laboratory or clinical proof.

### How does AI-driven drug discovery and development differ from a general AI in healthcare course?

It focuses on the medicine pipeline rather than hospital operations or diagnosis. A general healthcare AI course covers care delivery; this one covers targets, molecules, ADMET prediction and trial enrichment for R&D teams.

### What do you bring back from AI-driven drug discovery and development training?

You bring back a portfolio brief for your research unit. It records which models enter each pipeline stage, the evidence each needs, the decision gates and the people accountable.

## AI-Driven Drug Discovery and Development: The Way Forward

The AI Discovery Portfolio Brief first informs which pipeline stage receives a predictive model next and what validation it must pass before results influence a go or no-go decision. Discovery leads, clinical leads and informatics owners use it at portfolio reviews. After its first cycle, revisit how often model predictions agreed with assay and trial outcomes, and narrow each applicability domain accordingly.