

Global AI Drug Discovery Market 2026 by Company, Regions, Type and Application, Forecast to 2032

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Abstracts

According to our (Global Info Research) latest study, the global AI Drug Discovery market size was valued at US\$ 7131 million in 2025 and is forecast to a readjusted size of US\$ 47759 million by 2032 with a CAGR of 29.2% during review period.

AI Drug Discovery refers to the use of artificial intelligence (AI) technologies, machine learning (ML) algorithms, and big data analysis to accelerate drug discovery, design, screening, and optimization. The core advantage of AI drug discovery lies in its high data processing and pattern recognition capabilities, which can help identify potential drug candidates, predict biological activities, optimize preclinical drug effects, and shorten the drug development cycle. Common applications in AI drug discovery include target discovery, virtual screening, drug repurposing, molecular design, and clinical data analysis.

The upstream of the industry chain involves data resources and algorithm technologies, such as genomic data, protein structure databases, chemical libraries, and AI platforms. Downstream applications are concentrated in pharmaceutical companies, new drug R&D institutions, and contract research organizations (CROs), supporting drug discovery, target validation, drug repositioning, and personalized medicine design. Pharmaceutical companies leverage AI to shorten development cycles, reduce costs, and improve drug success rates. CROs utilize AI for compound screening, toxicity prediction, and clinical trial design, enhancing overall R&D efficiency.

Development trends include multimodal data integration, generative AI for drug design, AI-assisted clinical trial optimization, and precision medicine integration. Driving factors include high costs of traditional drug development, long R&D timelines, high clinical failure rates, and enhanced AI computational capabilities. Constraints include difficulty

in acquiring high-quality data, limited algorithm interpretability, regulatory uncertainties, and shortage of specialized talent. Overall industry gross margins are relatively high, typically ranging from 40% to 60%, driven by the added value of software and AI services to pharmaceutical companies and technological barriers.

This report is a detailed and comprehensive analysis for global AI Drug Discovery market. Both quantitative and qualitative analyses are presented by company, by region & country, by Type and by Application. As the market is constantly changing, this report explores the competition, supply and demand trends, as well as key factors that contribute to its changing demands across many markets. Company profiles and product examples of selected competitors, along with market share estimates of some of the selected leaders for the year 2025, are provided.

Key Features:

Global AI Drug Discovery market size and forecasts, in consumption value (\$ Million), 2021-2032

Global AI Drug Discovery market size and forecasts by region and country, in consumption value (\$ Million), 2021-2032

Global AI Drug Discovery market size and forecasts, by Type and by Application, in consumption value (\$ Million), 2021-2032

Global AI Drug Discovery market shares of main players, in revenue (\$ Million), 2021-2026

The Primary Objectives in This Report Are:

To determine the size of the total market opportunity of global and key countries

To assess the growth potential for AI Drug Discovery

To forecast future growth in each product and end-use market

To assess competitive factors affecting the marketplace

This report profiles key players in the global AI Drug Discovery market based on the

following parameters - company overview, revenue, gross margin, product portfolio, geographical presence, and key developments. Key companies covered as a part of this study include Recursion, Insilico Medicine, Schrödinger, DeepMind, Insitro, Generate Biomedicines, XtalPi, Relay Therapeutics, BenevolentAI, Roivant Sciences, etc.

This report also provides key insights about market drivers, restraints, opportunities, new product launches or approvals.

Market segmentation

AI Drug Discovery market is split by Type and by Application. For the period 2021-2032, the growth among segments provides accurate calculations and forecasts for Consumption Value by Type and by Application. This analysis can help you expand your business by targeting qualified niche markets.

Market segment by Type

Machine Learning Type

Deep Learning Type

Natural Language Processing Type

Data Mining Type

Market segment by Drug Type

Small Molecule Drugs

Biomacromolecules

Novel Therapies

Market segment by Computational Power

High-Performance Computing Type

Cloud Computing Type

Edge Computing Type

Market segment by Application

Target Discovery and Validation

Virtual Screening and Molecular Docking

Drug Repurposing and Precision Medicine

Clinical Data Analysis and Optimization

Market segment by players, this report covers

Recursion

Insilico Medicine

Schrödinger

DeepMind

Insitro

Generate Biomedicines

XtalPi

Relay Therapeutics

BenevolentAI

Roivant Sciences

Ginkgo Bioworks

Exscientia

Merck KGaA

Novartis

Biotus

Huazhi Bio

MindRank AI

Ubigene

WuXi AppTec

Market segment by regions, regional analysis covers

North America (United States, Canada and Mexico)

Europe (Germany, France, UK, Russia, Italy and Rest of Europe)

Asia-Pacific (China, Japan, South Korea, India, Southeast Asia and Rest of Asia-Pacific)

South America (Brazil, Rest of South America)

Middle East & Africa (Turkey, Saudi Arabia, UAE, Rest of Middle East & Africa)

The content of the study subjects, includes a total of 13 chapters:

Chapter 1, to describe AI Drug Discovery product scope, market overview, market estimation caveats and base year.

Chapter 2, to profile the top players of AI Drug Discovery, with revenue, gross margin, and global market share of AI Drug Discovery from 2021 to 2026.

Chapter 3, the AI Drug Discovery competitive situation, revenue, and global market share of top players are analyzed emphatically by landscape contrast.

Chapter 4 and 5, to segment the market size by Type and by Application, with consumption value and growth rate by Type, by Application, from 2021 to 2032.

Chapter 6, 7, 8, 9, and 10, to break the market size data at the country level, with revenue and market share for key countries in the world, from 2021 to 2026. and AI Drug Discovery market forecast, by regions, by Type and by Application, with consumption value, from 2027 to 2032.

Chapter 11, market dynamics, drivers, restraints, trends, Porters Five Forces analysis.

Chapter 12, the key raw materials and key suppliers, and industry chain of AI Drug Discovery.

Chapter 13, to describe AI Drug Discovery research findings and conclusion.

Contents

1 MARKET OVERVIEW

1.1 Product Overview and Scope

1.2 Market Estimation Caveats and Base Year

1.3 Classification of AI Drug Discovery by Type

1.3.1 Overview: Global AI Drug Discovery Market Size by Type: 2021 Versus 2025 Versus 2032

1.3.2 Global AI Drug Discovery Consumption Value Market Share by Type in 2025

1.3.3 Machine Learning Type

1.3.4 Deep Learning Type

1.3.5 Natural Language Processing Type

1.3.6 Data Mining Type

1.4 Classification of AI Drug Discovery by Drug Type

1.4.1 Overview: Global AI Drug Discovery Market Size by Drug Type: 2021 Versus 2025 Versus 2032

1.4.2 Global AI Drug Discovery Consumption Value Market Share by Drug Type in 2025

1.4.3 Small Molecule Drugs

1.4.4 Biomacromolecules

1.4.5 Novel Therapies

1.5 Classification of AI Drug Discovery by Computational Power

1.5.1 Overview: Global AI Drug Discovery Market Size by Computational Power: 2021 Versus 2025 Versus 2032

1.5.2 Global AI Drug Discovery Consumption Value Market Share by Computational Power in 2025

1.5.3 High-Performance Computing Type

1.5.4 Cloud Computing Type

1.5.5 Edge Computing Type

1.6 Global AI Drug Discovery Market by Application

1.6.1 Overview: Global AI Drug Discovery Market Size by Application: 2021 Versus 2025 Versus 2032

1.6.2 Target Discovery and Validation

1.6.3 Virtual Screening and Molecular Docking

1.6.4 Drug Repurposing and Precision Medicine

1.6.5 Clinical Data Analysis and Optimization

1.7 Global AI Drug Discovery Market Size & Forecast

1.8 Global AI Drug Discovery Market Size and Forecast by Region

- 1.8.1 Global AI Drug Discovery Market Size by Region: 2021 VS 2025 VS 2032
- 1.8.2 Global AI Drug Discovery Market Size by Region, (2021-2032)
- 1.8.3 North America AI Drug Discovery Market Size and Prospect (2021-2032)
- 1.8.4 Europe AI Drug Discovery Market Size and Prospect (2021-2032)
- 1.8.5 Asia-Pacific AI Drug Discovery Market Size and Prospect (2021-2032)
- 1.8.6 South America AI Drug Discovery Market Size and Prospect (2021-2032)
- 1.8.7 Middle East & Africa AI Drug Discovery Market Size and Prospect (2021-2032)

2 COMPANY PROFILES

2.1 Recursion

- 2.1.1 Recursion Details
- 2.1.2 Recursion Major Business
- 2.1.3 Recursion AI Drug Discovery Product and Solutions
- 2.1.4 Recursion AI Drug Discovery Revenue, Gross Margin and Market Share (2021-2026)
- 2.1.5 Recursion Recent Developments and Future Plans

2.2 Insilico Medicine

- 2.2.1 Insilico Medicine Details
- 2.2.2 Insilico Medicine Major Business
- 2.2.3 Insilico Medicine AI Drug Discovery Product and Solutions
- 2.2.4 Insilico Medicine AI Drug Discovery Revenue, Gross Margin and Market Share (2021-2026)
- 2.2.5 Insilico Medicine Recent Developments and Future Plans

2.3 Schrödinger

- 2.3.1 Schrödinger Details
- 2.3.2 Schrödinger Major Business
- 2.3.3 Schrödinger AI Drug Discovery Product and Solutions
- 2.3.4 Schrödinger AI Drug Discovery Revenue, Gross Margin and Market Share (2021-2026)
- 2.3.5 Schrödinger Recent Developments and Future Plans

2.4 DeepMind

- 2.4.1 DeepMind Details
- 2.4.2 DeepMind Major Business
- 2.4.3 DeepMind AI Drug Discovery Product and Solutions
- 2.4.4 DeepMind AI Drug Discovery Revenue, Gross Margin and Market Share (2021-2026)
- 2.4.5 DeepMind Recent Developments and Future Plans

2.5 Insitro

- 2.5.1 Insitro Details
- 2.5.2 Insitro Major Business
- 2.5.3 Insitro AI Drug Discovery Product and Solutions
- 2.5.4 Insitro AI Drug Discovery Revenue, Gross Margin and Market Share (2021-2026)
- 2.5.5 Insitro Recent Developments and Future Plans
- 2.6 Generate Biomedicines
 - 2.6.1 Generate Biomedicines Details
 - 2.6.2 Generate Biomedicines Major Business
 - 2.6.3 Generate Biomedicines AI Drug Discovery Product and Solutions
 - 2.6.4 Generate Biomedicines AI Drug Discovery Revenue, Gross Margin and Market Share (2021-2026)
 - 2.6.5 Generate Biomedicines Recent Developments and Future Plans
- 2.7 XtalPi
 - 2.7.1 XtalPi Details
 - 2.7.2 XtalPi Major Business
 - 2.7.3 XtalPi AI Drug Discovery Product and Solutions
 - 2.7.4 XtalPi AI Drug Discovery Revenue, Gross Margin and Market Share (2021-2026)
 - 2.7.5 XtalPi Recent Developments and Future Plans
- 2.8 Relay Therapeutics
 - 2.8.1 Relay Therapeutics Details
 - 2.8.2 Relay Therapeutics Major Business
 - 2.8.3 Relay Therapeutics AI Drug Discovery Product and Solutions
 - 2.8.4 Relay Therapeutics AI Drug Discovery Revenue, Gross Margin and Market Share (2021-2026)
 - 2.8.5 Relay Therapeutics Recent Developments and Future Plans
- 2.9 BenevolentAI
 - 2.9.1 BenevolentAI Details
 - 2.9.2 BenevolentAI Major Business
 - 2.9.3 BenevolentAI AI Drug Discovery Product and Solutions
 - 2.9.4 BenevolentAI AI Drug Discovery Revenue, Gross Margin and Market Share (2021-2026)
 - 2.9.5 BenevolentAI Recent Developments and Future Plans
- 2.10 Roivant Sciences
 - 2.10.1 Roivant Sciences Details
 - 2.10.2 Roivant Sciences Major Business
 - 2.10.3 Roivant Sciences AI Drug Discovery Product and Solutions
 - 2.10.4 Roivant Sciences AI Drug Discovery Revenue, Gross Margin and Market Share (2021-2026)
 - 2.10.5 Roivant Sciences Recent Developments and Future Plans

2.11 Ginkgo Bioworks

2.11.1 Ginkgo Bioworks Details

2.11.2 Ginkgo Bioworks Major Business

2.11.3 Ginkgo Bioworks AI Drug Discovery Product and Solutions

2.11.4 Ginkgo Bioworks AI Drug Discovery Revenue, Gross Margin and Market Share (2021-2026)

2.11.5 Ginkgo Bioworks Recent Developments and Future Plans

2.12 Exscientia

2.12.1 Exscientia Details

2.12.2 Exscientia Major Business

2.12.3 Exscientia AI Drug Discovery Product and Solutions

2.12.4 Exscientia AI Drug Discovery Revenue, Gross Margin and Market Share (2021-2026)

2.12.5 Exscientia Recent Developments and Future Plans

2.13 Merck KGaA

2.13.1 Merck KGaA Details

2.13.2 Merck KGaA Major Business

2.13.3 Merck KGaA AI Drug Discovery Product and Solutions

2.13.4 Merck KGaA AI Drug Discovery Revenue, Gross Margin and Market Share (2021-2026)

2.13.5 Merck KGaA Recent Developments and Future Plans

2.14 Novartis

2.14.1 Novartis Details

2.14.2 Novartis Major Business

2.14.3 Novartis AI Drug Discovery Product and Solutions

2.14.4 Novartis AI Drug Discovery Revenue, Gross Margin and Market Share (2021-2026)

2.14.5 Novartis Recent Developments and Future Plans

2.15 Biotus

2.15.1 Biotus Details

2.15.2 Biotus Major Business

2.15.3 Biotus AI Drug Discovery Product and Solutions

2.15.4 Biotus AI Drug Discovery Revenue, Gross Margin and Market Share (2021-2026)

2.15.5 Biotus Recent Developments and Future Plans

2.16 Huazhi Bio

2.16.1 Huazhi Bio Details

2.16.2 Huazhi Bio Major Business

2.16.3 Huazhi Bio AI Drug Discovery Product and Solutions

2.16.4 Huazhi Bio AI Drug Discovery Revenue, Gross Margin and Market Share (2021-2026)

2.16.5 Huazhi Bio Recent Developments and Future Plans

2.17 MindRank AI

2.17.1 MindRank AI Details

2.17.2 MindRank AI Major Business

2.17.3 MindRank AI AI Drug Discovery Product and Solutions

2.17.4 MindRank AI AI Drug Discovery Revenue, Gross Margin and Market Share (2021-2026)

2.17.5 MindRank AI Recent Developments and Future Plans

2.18 Ubigene

2.18.1 Ubigene Details

2.18.2 Ubigene Major Business

2.18.3 Ubigene AI Drug Discovery Product and Solutions

2.18.4 Ubigene AI Drug Discovery Revenue, Gross Margin and Market Share (2021-2026)

2.18.5 Ubigene Recent Developments and Future Plans

2.19 WuXi AppTec

2.19.1 WuXi AppTec Details

2.19.2 WuXi AppTec Major Business

2.19.3 WuXi AppTec AI Drug Discovery Product and Solutions

2.19.4 WuXi AppTec AI Drug Discovery Revenue, Gross Margin and Market Share (2021-2026)

2.19.5 WuXi AppTec Recent Developments and Future Plans

3 MARKET COMPETITION, BY PLAYERS

3.1 Global AI Drug Discovery Revenue and Share by Players (2021-2026)

3.2 Market Share Analysis (2025)

3.2.1 Market Share of AI Drug Discovery by Company Revenue

3.2.2 Top 3 AI Drug Discovery Players Market Share in 2025

3.2.3 Top 6 AI Drug Discovery Players Market Share in 2025

3.3 AI Drug Discovery Market: Overall Company Footprint Analysis

3.3.1 AI Drug Discovery Market: Region Footprint

3.3.2 AI Drug Discovery Market: Company Product Type Footprint

3.3.3 AI Drug Discovery Market: Company Product Application Footprint

3.4 New Market Entrants and Barriers to Market Entry

3.5 Mergers, Acquisition, Agreements, and Collaborations

4 MARKET SIZE SEGMENT BY TYPE

4.1 Global AI Drug Discovery Consumption Value and Market Share by Type (2021-2026)

4.2 Global AI Drug Discovery Market Forecast by Type (2027-2032)

5 MARKET SIZE SEGMENT BY APPLICATION

5.1 Global AI Drug Discovery Consumption Value Market Share by Application (2021-2026)

5.2 Global AI Drug Discovery Market Forecast by Application (2027-2032)

6 NORTH AMERICA

6.1 North America AI Drug Discovery Consumption Value by Type (2021-2032)

6.2 North America AI Drug Discovery Market Size by Application (2021-2032)

6.3 North America AI Drug Discovery Market Size by Country

6.3.1 North America AI Drug Discovery Consumption Value by Country (2021-2032)

6.3.2 United States AI Drug Discovery Market Size and Forecast (2021-2032)

6.3.3 Canada AI Drug Discovery Market Size and Forecast (2021-2032)

6.3.4 Mexico AI Drug Discovery Market Size and Forecast (2021-2032)

7 EUROPE

7.1 Europe AI Drug Discovery Consumption Value by Type (2021-2032)

7.2 Europe AI Drug Discovery Consumption Value by Application (2021-2032)

7.3 Europe AI Drug Discovery Market Size by Country

7.3.1 Europe AI Drug Discovery Consumption Value by Country (2021-2032)

7.3.2 Germany AI Drug Discovery Market Size and Forecast (2021-2032)

7.3.3 France AI Drug Discovery Market Size and Forecast (2021-2032)

7.3.4 United Kingdom AI Drug Discovery Market Size and Forecast (2021-2032)

7.3.5 Russia AI Drug Discovery Market Size and Forecast (2021-2032)

7.3.6 Italy AI Drug Discovery Market Size and Forecast (2021-2032)

8 ASIA-PACIFIC

8.1 Asia-Pacific AI Drug Discovery Consumption Value by Type (2021-2032)

8.2 Asia-Pacific AI Drug Discovery Consumption Value by Application (2021-2032)

8.3 Asia-Pacific AI Drug Discovery Market Size by Region

- 8.3.1 Asia-Pacific AI Drug Discovery Consumption Value by Region (2021-2032)
- 8.3.2 China AI Drug Discovery Market Size and Forecast (2021-2032)
- 8.3.3 Japan AI Drug Discovery Market Size and Forecast (2021-2032)
- 8.3.4 South Korea AI Drug Discovery Market Size and Forecast (2021-2032)
- 8.3.5 India AI Drug Discovery Market Size and Forecast (2021-2032)
- 8.3.6 Southeast Asia AI Drug Discovery Market Size and Forecast (2021-2032)
- 8.3.7 Australia AI Drug Discovery Market Size and Forecast (2021-2032)

9 SOUTH AMERICA

- 9.1 South America AI Drug Discovery Consumption Value by Type (2021-2032)
- 9.2 South America AI Drug Discovery Consumption Value by Application (2021-2032)
- 9.3 South America AI Drug Discovery Market Size by Country
 - 9.3.1 South America AI Drug Discovery Consumption Value by Country (2021-2032)
 - 9.3.2 Brazil AI Drug Discovery Market Size and Forecast (2021-2032)
 - 9.3.3 Argentina AI Drug Discovery Market Size and Forecast (2021-2032)

10 MIDDLE EAST & AFRICA

- 10.1 Middle East & Africa AI Drug Discovery Consumption Value by Type (2021-2032)
- 10.2 Middle East & Africa AI Drug Discovery Consumption Value by Application (2021-2032)
- 10.3 Middle East & Africa AI Drug Discovery Market Size by Country
 - 10.3.1 Middle East & Africa AI Drug Discovery Consumption Value by Country (2021-2032)
 - 10.3.2 Turkey AI Drug Discovery Market Size and Forecast (2021-2032)
 - 10.3.3 Saudi Arabia AI Drug Discovery Market Size and Forecast (2021-2032)
 - 10.3.4 UAE AI Drug Discovery Market Size and Forecast (2021-2032)

11 MARKET DYNAMICS

- 11.1 AI Drug Discovery Market Drivers
- 11.2 AI Drug Discovery Market Restraints
- 11.3 AI Drug Discovery Trends Analysis
- 11.4 Porters Five Forces Analysis
 - 11.4.1 Threat of New Entrants
 - 11.4.2 Bargaining Power of Suppliers
 - 11.4.3 Bargaining Power of Buyers
 - 11.4.4 Threat of Substitutes

11.4.5 Competitive Rivalry

12 INDUSTRY CHAIN ANALYSIS

12.1 AI Drug Discovery Industry Chain

12.2 AI Drug Discovery Upstream Analysis

12.3 AI Drug Discovery Midstream Analysis

12.4 AI Drug Discovery Downstream Analysis

13 RESEARCH FINDINGS AND CONCLUSION

14 APPENDIX

14.1 Methodology

14.2 Research Process and Data Source

14.3 Disclaimer

List Of Tables

LIST OF TABLES

Table 1. Global AI Drug Discovery Consumption Value by Type, (USD Million), 2021 & 2025 & 2032

Table 2. Global AI Drug Discovery Consumption Value by Drug Type, (USD Million), 2021 & 2025 & 2032

Table 3. Global AI Drug Discovery Consumption Value by Computational Power, (USD Million), 2021 & 2025 & 2032

Table 4. Global AI Drug Discovery Consumption Value by Application, (USD Million), 2021 & 2025 & 2032

Table 5. Global AI Drug Discovery Consumption Value by Region (2021-2026) & (USD Million)

Table 6. Global AI Drug Discovery Consumption Value by Region (2027-2032) & (USD Million)

Table 7. Recursion Company Information, Head Office, and Major Competitors

Table 8. Recursion Major Business

Table 9. Recursion AI Drug Discovery Product and Solutions

Table 10. Recursion AI Drug Discovery Revenue (USD Million), Gross Margin and Market Share (2021-2026)

Table 11. Recursion Recent Developments and Future Plans

Table 12. Insilico Medicine Company Information, Head Office, and Major Competitors

Table 13. Insilico Medicine Major Business

Table 14. Insilico Medicine AI Drug Discovery Product and Solutions

Table 15. Insilico Medicine AI Drug Discovery Revenue (USD Million), Gross Margin and Market Share (2021-2026)

Table 16. Insilico Medicine Recent Developments and Future Plans

Table 17. Schrödinger Company Information, Head Office, and Major Competitors

Table 18. Schrödinger Major Business

Table 19. Schrödinger AI Drug Discovery Product and Solutions

Table 20. Schrödinger AI Drug Discovery Revenue (USD Million), Gross Margin and Market Share (2021-2026)

Table 21. DeepMind Company Information, Head Office, and Major Competitors

Table 22. DeepMind Major Business

Table 23. DeepMind AI Drug Discovery Product and Solutions

Table 24. DeepMind AI Drug Discovery Revenue (USD Million), Gross Margin and Market Share (2021-2026)

Table 25. DeepMind Recent Developments and Future Plans

Table 26. Insitro Company Information, Head Office, and Major Competitors
Table 27. Insitro Major Business
Table 28. Insitro AI Drug Discovery Product and Solutions
Table 29. Insitro AI Drug Discovery Revenue (USD Million), Gross Margin and Market Share (2021-2026)
Table 30. Insitro Recent Developments and Future Plans
Table 31. Generate Biomedicines Company Information, Head Office, and Major Competitors
Table 32. Generate Biomedicines Major Business
Table 33. Generate Biomedicines AI Drug Discovery Product and Solutions
Table 34. Generate Biomedicines AI Drug Discovery Revenue (USD Million), Gross Margin and Market Share (2021-2026)
Table 35. Generate Biomedicines Recent Developments and Future Plans
Table 36. XtalPi Company Information, Head Office, and Major Competitors
Table 37. XtalPi Major Business
Table 38. XtalPi AI Drug Discovery Product and Solutions
Table 39. XtalPi AI Drug Discovery Revenue (USD Million), Gross Margin and Market Share (2021-2026)
Table 40. XtalPi Recent Developments and Future Plans
Table 41. Relay Therapeutics Company Information, Head Office, and Major Competitors
Table 42. Relay Therapeutics Major Business
Table 43. Relay Therapeutics AI Drug Discovery Product and Solutions
Table 44. Relay Therapeutics AI Drug Discovery Revenue (USD Million), Gross Margin and Market Share (2021-2026)
Table 45. Relay Therapeutics Recent Developments and Future Plans
Table 46. BenevolentAI Company Information, Head Office, and Major Competitors
Table 47. BenevolentAI Major Business
Table 48. BenevolentAI AI Drug Discovery Product and Solutions
Table 49. BenevolentAI AI Drug Discovery Revenue (USD Million), Gross Margin and Market Share (2021-2026)
Table 50. BenevolentAI Recent Developments and Future Plans
Table 51. Roivant Sciences Company Information, Head Office, and Major Competitors
Table 52. Roivant Sciences Major Business
Table 53. Roivant Sciences AI Drug Discovery Product and Solutions
Table 54. Roivant Sciences AI Drug Discovery Revenue (USD Million), Gross Margin and Market Share (2021-2026)
Table 55. Roivant Sciences Recent Developments and Future Plans
Table 56. Ginkgo Bioworks Company Information, Head Office, and Major Competitors

Table 57. Ginkgo Bioworks Major Business
Table 58. Ginkgo Bioworks AI Drug Discovery Product and Solutions
Table 59. Ginkgo Bioworks AI Drug Discovery Revenue (USD Million), Gross Margin and Market Share (2021-2026)
Table 60. Ginkgo Bioworks Recent Developments and Future Plans
Table 61. Exscientia Company Information, Head Office, and Major Competitors
Table 62. Exscientia Major Business
Table 63. Exscientia AI Drug Discovery Product and Solutions
Table 64. Exscientia AI Drug Discovery Revenue (USD Million), Gross Margin and Market Share (2021-2026)
Table 65. Exscientia Recent Developments and Future Plans
Table 66. Merck KGaA Company Information, Head Office, and Major Competitors
Table 67. Merck KGaA Major Business
Table 68. Merck KGaA AI Drug Discovery Product and Solutions
Table 69. Merck KGaA AI Drug Discovery Revenue (USD Million), Gross Margin and Market Share (2021-2026)
Table 70. Merck KGaA Recent Developments and Future Plans
Table 71. Novartis Company Information, Head Office, and Major Competitors
Table 72. Novartis Major Business
Table 73. Novartis AI Drug Discovery Product and Solutions
Table 74. Novartis AI Drug Discovery Revenue (USD Million), Gross Margin and Market Share (2021-2026)
Table 75. Novartis Recent Developments and Future Plans
Table 76. Biotus Company Information, Head Office, and Major Competitors
Table 77. Biotus Major Business
Table 78. Biotus AI Drug Discovery Product and Solutions
Table 79. Biotus AI Drug Discovery Revenue (USD Million), Gross Margin and Market Share (2021-2026)
Table 80. Biotus Recent Developments and Future Plans
Table 81. Huazhi Bio Company Information, Head Office, and Major Competitors
Table 82. Huazhi Bio Major Business
Table 83. Huazhi Bio AI Drug Discovery Product and Solutions
Table 84. Huazhi Bio AI Drug Discovery Revenue (USD Million), Gross Margin and Market Share (2021-2026)
Table 85. Huazhi Bio Recent Developments and Future Plans
Table 86. MindRank AI Company Information, Head Office, and Major Competitors
Table 87. MindRank AI Major Business
Table 88. MindRank AI AI Drug Discovery Product and Solutions
Table 89. MindRank AI AI Drug Discovery Revenue (USD Million), Gross Margin and

Market Share (2021-2026)

Table 90. MindRank AI Recent Developments and Future Plans

Table 91. Ubigen Company Information, Head Office, and Major Competitors

Table 92. Ubigen Major Business

Table 93. Ubigen AI Drug Discovery Product and Solutions

Table 94. Ubigen AI Drug Discovery Revenue (USD Million), Gross Margin and Market Share (2021-2026)

Table 95. Ubigen Recent Developments and Future Plans

Table 96. WuXi AppTec Company Information, Head Office, and Major Competitors

Table 97. WuXi AppTec Major Business

Table 98. WuXi AppTec AI Drug Discovery Product and Solutions

Table 99. WuXi AppTec AI Drug Discovery Revenue (USD Million), Gross Margin and Market Share (2021-2026)

Table 100. WuXi AppTec Recent Developments and Future Plans

Table 101. Global AI Drug Discovery Revenue (USD Million) by Players (2021-2026)

Table 102. Global AI Drug Discovery Revenue Share by Players (2021-2026)

Table 103. Breakdown of AI Drug Discovery by Company Type (Tier 1, Tier 2, and Tier 3)

Table 104. Market Position of Players in AI Drug Discovery, (Tier 1, Tier 2, and Tier 3), Based on Revenue in 2025

Table 105. Head Office of Key AI Drug Discovery Players

Table 106. AI Drug Discovery Market: Company Product Type Footprint

Table 107. AI Drug Discovery Market: Company Product Application Footprint

Table 108. AI Drug Discovery New Market Entrants and Barriers to Market Entry

Table 109. AI Drug Discovery Mergers, Acquisition, Agreements, and Collaborations

Table 110. Global AI Drug Discovery Consumption Value (USD Million) by Type (2021-2026)

Table 111. Global AI Drug Discovery Consumption Value Share by Type (2021-2026)

Table 112. Global AI Drug Discovery Consumption Value Forecast by Type (2027-2032)

Table 113. Global AI Drug Discovery Consumption Value by Application (2021-2026)

Table 114. Global AI Drug Discovery Consumption Value Forecast by Application (2027-2032)

Table 115. North America AI Drug Discovery Consumption Value by Type (2021-2026) & (USD Million)

Table 116. North America AI Drug Discovery Consumption Value by Type (2027-2032) & (USD Million)

Table 117. North America AI Drug Discovery Consumption Value by Application (2021-2026) & (USD Million)

Table 118. North America AI Drug Discovery Consumption Value by Application

(2027-2032) & (USD Million)

Table 119. North America AI Drug Discovery Consumption Value by Country

(2021-2026) & (USD Million)

Table 120. North America AI Drug Discovery Consumption Value by Country

(2027-2032) & (USD Million)

Table 121. Europe AI Drug Discovery Consumption Value by Type (2021-2026) & (USD Million)

Table 122. Europe AI Drug Discovery Consumption Value by Type (2027-2032) & (USD Million)

Table 123. Europe AI Drug Discovery Consumption Value by Application (2021-2026) & (USD Million)

Table 124. Europe AI Drug Discovery Consumption Value by Application (2027-2032) & (USD Million)

Table 125. Europe AI Drug Discovery Consumption Value by Country (2021-2026) & (USD Million)

Table 126. Europe AI Drug Discovery Consumption Value by Country (2027-2032) & (USD Million)

Table 127. Asia-Pacific AI Drug Discovery Consumption Value by Type (2021-2026) & (USD Million)

Table 128. Asia-Pacific AI Drug Discovery Consumption Value by Type (2027-2032) & (USD Million)

Table 129. Asia-Pacific AI Drug Discovery Consumption Value by Application (2021-2026) & (USD Million)

Table 130. Asia-Pacific AI Drug Discovery Consumption Value by Application (2027-2032) & (USD Million)

Table 131. Asia-Pacific AI Drug Discovery Consumption Value by Region (2021-2026) & (USD Million)

Table 132. Asia-Pacific AI Drug Discovery Consumption Value by Region (2027-2032) & (USD Million)

Table 133. South America AI Drug Discovery Consumption Value by Type (2021-2026) & (USD Million)

Table 134. South America AI Drug Discovery Consumption Value by Type (2027-2032) & (USD Million)

Table 135. South America AI Drug Discovery Consumption Value by Application (2021-2026) & (USD Million)

Table 136. South America AI Drug Discovery Consumption Value by Application (2027-2032) & (USD Million)

Table 137. South America AI Drug Discovery Consumption Value by Country (2021-2026) & (USD Million)

Table 138. South America AI Drug Discovery Consumption Value by Country
(2027-2032) & (USD Million)

Table 139. Middle East & Africa AI Drug Discovery Consumption Value by Type
(2021-2026) & (USD Million)

Table 140. Middle East & Africa AI Drug Discovery Consumption Value by Type
(2027-2032) & (USD Million)

Table 141. Middle East & Africa AI Drug Discovery Consumption Value by Application
(2021-2026) & (USD Million)

Table 142. Middle East & Africa AI Drug Discovery Consumption Value by Application
(2027-2032) & (USD Million)

Table 143. Middle East & Africa AI Drug Discovery Consumption Value by Country
(2021-2026) & (USD Million)

Table 144. Middle East & Africa AI Drug Discovery Consumption Value by Country
(2027-2032) & (USD Million)

Table 145. Global Key Players of AI Drug Discovery Upstream (Raw Materials)

Table 146. Global AI Drug Discovery Typical Customers

List Of Figures

LIST OF FIGURES

Figure 1. AI Drug Discovery Picture

Figure 2. Global AI Drug Discovery Consumption Value by Type, (USD Million), 2021 & 2025 & 2032

Figure 3. Global AI Drug Discovery Consumption Value Market Share by Type in 2025

Figure 4. Machine Learning Type

Figure 5. Deep Learning Type

Figure 6. Natural Language Processing Type

Figure 7. Data Mining Type

Figure 8. Global AI Drug Discovery Consumption Value by Drug Type, (USD Million), 2021 & 2025 & 2032

Figure 9. Global AI Drug Discovery Consumption Value Market Share by Drug Type in 2025

Figure 10. Small Molecule Drugs

Figure 11. Biomacromolecules

Figure 12. Novel Therapies

Figure 13. Global AI Drug Discovery Consumption Value by Computational Power, (USD Million), 2021 & 2025 & 2032

Figure 14. Global AI Drug Discovery Consumption Value Market Share by Computational Power in 2025

Figure 15. High-Performance Computing Type

Figure 16. Cloud Computing Type

Figure 17. Edge Computing Type

Figure 18. Global AI Drug Discovery Consumption Value by Application, (USD Million), 2021 & 2025 & 2032

Figure 19. AI Drug Discovery Consumption Value Market Share by Application in 2025

Figure 20. Target Discovery and Validation Picture

Figure 21. Virtual Screening and Molecular Docking Picture

Figure 22. Drug Repurposing and Precision Medicine Picture

Figure 23. Clinical Data Analysis and Optimization Picture

Figure 24. Global AI Drug Discovery Consumption Value, (USD Million): 2021 & 2025 & 2032

Figure 25. Global AI Drug Discovery Consumption Value and Forecast (2021-2032) & (USD Million)

Figure 26. Global Market AI Drug Discovery Consumption Value (USD Million) Comparison by Region (2021 VS 2025 VS 2032)

Figure 27. Global AI Drug Discovery Consumption Value Market Share by Region (2021-2032)

Figure 28. Global AI Drug Discovery Consumption Value Market Share by Region in 2025

Figure 29. North America AI Drug Discovery Consumption Value (2021-2032) & (USD Million)

Figure 30. Europe AI Drug Discovery Consumption Value (2021-2032) & (USD Million)

Figure 31. Asia-Pacific AI Drug Discovery Consumption Value (2021-2032) & (USD Million)

Figure 32. South America AI Drug Discovery Consumption Value (2021-2032) & (USD Million)

Figure 33. Middle East & Africa AI Drug Discovery Consumption Value (2021-2032) & (USD Million)

Figure 34. Company Three Recent Developments and Future Plans

Figure 35. Global AI Drug Discovery Revenue Share by Players in 2025

Figure 36. AI Drug Discovery Market Share by Company Type (Tier 1, Tier 2, and Tier 3) in 2025

Figure 37. Market Share of AI Drug Discovery by Player Revenue in 2025

Figure 38. Top 3 AI Drug Discovery Players Market Share in 2025

Figure 39. Top 6 AI Drug Discovery Players Market Share in 2025

Figure 40. Global AI Drug Discovery Consumption Value Share by Type (2021-2026)

Figure 41. Global AI Drug Discovery Market Share Forecast by Type (2027-2032)

Figure 42. Global AI Drug Discovery Consumption Value Share by Application (2021-2026)

Figure 43. Global AI Drug Discovery Market Share Forecast by Application (2027-2032)

Figure 44. North America AI Drug Discovery Consumption Value Market Share by Type (2021-2032)

Figure 45. North America AI Drug Discovery Consumption Value Market Share by Application (2021-2032)

Figure 46. North America AI Drug Discovery Consumption Value Market Share by Country (2021-2032)

Figure 47. United States AI Drug Discovery Consumption Value (2021-2032) & (USD Million)

Figure 48. Canada AI Drug Discovery Consumption Value (2021-2032) & (USD Million)

Figure 49. Mexico AI Drug Discovery Consumption Value (2021-2032) & (USD Million)

Figure 50. Europe AI Drug Discovery Consumption Value Market Share by Type (2021-2032)

Figure 51. Europe AI Drug Discovery Consumption Value Market Share by Application (2021-2032)

Figure 52. Europe AI Drug Discovery Consumption Value Market Share by Country (2021-2032)

Figure 53. Germany AI Drug Discovery Consumption Value (2021-2032) & (USD Million)

Figure 54. France AI Drug Discovery Consumption Value (2021-2032) & (USD Million)

Figure 55. United Kingdom AI Drug Discovery Consumption Value (2021-2032) & (USD Million)

Figure 56. Russia AI Drug Discovery Consumption Value (2021-2032) & (USD Million)

Figure 57. Italy AI Drug Discovery Consumption Value (2021-2032) & (USD Million)

Figure 58. Asia-Pacific AI Drug Discovery Consumption Value Market Share by Type (2021-2032)

Figure 59. Asia-Pacific AI Drug Discovery Consumption Value Market Share by Application (2021-2032)

Figure 60. Asia-Pacific AI Drug Discovery Consumption Value Market Share by Region (2021-2032)

Figure 61. China AI Drug Discovery Consumption Value (2021-2032) & (USD Million)

Figure 62. Japan AI Drug Discovery Consumption Value (2021-2032) & (USD Million)

Figure 63. South Korea AI Drug Discovery Consumption Value (2021-2032) & (USD Million)

Figure 64. India AI Drug Discovery Consumption Value (2021-2032) & (USD Million)

Figure 65. Southeast Asia AI Drug Discovery Consumption Value (2021-2032) & (USD Million)

Figure 66. Australia AI Drug Discovery Consumption Value (2021-2032) & (USD Million)

Figure 67. South America AI Drug Discovery Consumption Value Market Share by Type (2021-2032)

Figure 68. South America AI Drug Discovery Consumption Value Market Share by Application (2021-2032)

Figure 69. South America AI Drug Discovery Consumption Value Market Share by Country (2021-2032)

Figure 70. Brazil AI Drug Discovery Consumption Value (2021-2032) & (USD Million)

Figure 71. Argentina AI Drug Discovery Consumption Value (2021-2032) & (USD Million)

Figure 72. Middle East & Africa AI Drug Discovery Consumption Value Market Share by Type (2021-2032)

Figure 73. Middle East & Africa AI Drug Discovery Consumption Value Market Share by Application (2021-2032)

Figure 74. Middle East & Africa AI Drug Discovery Consumption Value Market Share by Country (2021-2032)

Figure 75. Turkey AI Drug Discovery Consumption Value (2021-2032) & (USD Million)

Figure 76. Saudi Arabia AI Drug Discovery Consumption Value (2021-2032) & (USD Million)

Figure 77. UAE AI Drug Discovery Consumption Value (2021-2032) & (USD Million)

Figure 78. AI Drug Discovery Market Drivers

Figure 79. AI Drug Discovery Market Restraints

Figure 80. AI Drug Discovery Market Trends

Figure 81. Porters Five Forces Analysis

Figure 82. AI Drug Discovery Industrial Chain

Figure 83. Methodology

Figure 84. Research Process and Data Source

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