

Global Molecular Docking and Virtual Screening Software Supply, Demand and Key Producers, 2026-2032

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Abstracts

The global Molecular Docking and Virtual Screening Software market size is expected to reach \$ 1654 million by 2032, rising at a market growth of 14.5% CAGR during the forecast period (2026-2032).

Molecular docking and virtual screening software refers to computer-aided drug design tools used to predict interactions among small molecules, fragments, peptides, or protein complexes. It typically supports receptor preparation, ligand conformation generation, binding-site setup, conformational sampling, scoring, ranking, and visualization to screen large compound libraries for potential hits, with optional capabilities such as pharmacophore screening, shape similarity, induced-fit docking, covalent docking, and MM/GBSA or FEP rescoring. Deployment formats include desktop software, server or HPC clusters, cloud SaaS platforms, and API toolkits, mainly serving new drug discovery, drug repurposing, and lead optimization. The blended gross margin is approximately 75%.

Demand is mainly driven by early-stage innovative drug discovery, AI-enabled drug design platforms, computational chemistry services at CROs, drug repurposing, and academic research. As more protein structures become available, commercial compound libraries expand, and R&D teams seek higher pre-experimental screening efficiency, molecular docking and virtual screening software is moving from an expert-only tool to a standardized platform shared across project teams.

Product upgrades are centered on more complete workflows and higher computational efficiency. Established vendors maintain barriers through physics-based scoring functions, graphical modeling environments, and validated pharmaceutical use cases,

while newer entrants emphasize GPU acceleration, cloud elasticity, AI-based pose prediction, automated data pipelines, and API integration. Buyers increasingly evaluate not only docking accuracy, but also protein and ligand preparation, batch job management, rescoring, traceable reporting, data security, and connectivity with ELN, LIMS, ADMET, and FEP platforms.

Regional demand remains concentrated among large pharmaceutical companies, biotech firms, and specialist CROs in North America and Europe, while China, India, and Singapore are growing faster due to the expansion of local AI drug discovery and CXO capabilities. Key risks include wet-lab validation conversion, pricing pressure from open-source tools, customer data security, cloud computing cost, and model generalization; opportunities lie in enterprise private deployment, ultra-large-scale screening, fragment and covalent drug design, DEL or automated synthesis integration, and target-family-specific solutions.

This report studies the global Molecular Docking and Virtual Screening Software demand, key companies, and key regions.

This report is a detailed and comprehensive analysis of the world market for Molecular Docking and Virtual Screening Software, and provides market size (US\$ million) and Year-over-Year (YoY) growth, considering 2025 as the base year. This report explores demand trends and competition, as well as details the characteristics of Molecular Docking and Virtual Screening Software that contribute to its increasing demand across many markets.

Highlights and key features of the study

Global Molecular Docking and Virtual Screening Software total market, 2021-2032, (USD Million)

Global Molecular Docking and Virtual Screening Software total market by region & country, CAGR, 2021-2032, (USD Million)

U.S. VS China: Molecular Docking and Virtual Screening Software total market, key domestic companies, and share, (USD Million)

Global Molecular Docking and Virtual Screening Software revenue by player, revenue and market share 2021-2026, (USD Million)

Global Molecular Docking and Virtual Screening Software total market by Type, CAGR, 2021-2032, (USD Million)

Global Molecular Docking and Virtual Screening Software total market by Application, CAGR, 2021-2032, (USD Million)

This report profiles major players in the global Molecular Docking and Virtual Screening Software 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 Schrödinger, Dassault Systèmes, Chemical Computing Group, OpenEye Cadence Molecular Sciences, Cambridge Crystallographic Data Centre, Cresset, BioSolveIT, Molsoft, Molecular Discovery, DP Technology, etc.

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

Stakeholders would have ease in decision-making through various strategy matrices used in analyzing the world Molecular Docking and Virtual Screening Software market

Detailed Segmentation:

Each section contains quantitative market data including market by value (US\$ Millions), by player, by regions, by Type, and by Application. Data is given for the years 2021-2032 by year with 2025 as the base year, 2026 as the estimate year, and 2027-2032 as the forecast year.

Global Molecular Docking and Virtual Screening Software Market, By Region:

United States

China

Europe

Japan

South Korea

ASEAN

India

Rest of World

Global Molecular Docking and Virtual Screening Software Market, Segmentation by Type:

- Structure-Based Docking Software
- Ligand-Based Screening Software
- Pharmacophore Screening Software
- Shape and Electrostatic Similarity Software
- AI-Assisted Docking Software

Global Molecular Docking and Virtual Screening Software Market, Segmentation by Deployment Mode:

- Desktop Workstation Software
- Server or HPC Software
- Cloud SaaS Platform
- API or Toolkit Software
- Hybrid Deployment Software

Global Molecular Docking and Virtual Screening Software Market, Segmentation by Supported Molecule Type:

- Small Molecule Docking Software
- Fragment Docking Software
- Peptide Docking Software

Covalent Ligand Docking Software

Protein-Protein Docking Software

Global Molecular Docking and Virtual Screening Software Market, Segmentation by License Model:

Perpetual License Software

Subscription License Software

Cloud Usage-Based Software

Academic or Free Software

Enterprise Site License Software

Global Molecular Docking and Virtual Screening Software Market, Segmentation by Application:

Hit Discovery

Lead Optimization

Drug Repurposing

Fragment-Based Drug Design

Target Validation and Mechanism Study

Teaching and Academic Research

Companies Profiled:

Schrödinger

Dassault Syst?mes

Chemical Computing Group

OpenEye Cadence Molecular Sciences

Cambridge Crystallographic Data Centre

Cresset

BioSolveIT

Molsoft

Molecular Discovery

DP Technology

XtalPi

Key Questions Answered

1. How big is the global Molecular Docking and Virtual Screening Software market?
2. What is the demand of the global Molecular Docking and Virtual Screening Software market?
3. What is the year over year growth of the global Molecular Docking and Virtual Screening Software market?
4. What is the total value of the global Molecular Docking and Virtual Screening Software market?
5. Who are the Major Players in the global Molecular Docking and Virtual Screening Software market?
6. What are the growth factors driving the market demand?

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