

Global Molecular Docking and Virtual Screening Software 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 Molecular Docking and Virtual Screening Software market size was valued at US\$ 638 million in 2025 and is forecast to a readjusted size of US\$ 1654 million by 2032 with a CAGR of 14.5% during review period.

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 is a detailed and comprehensive analysis for global Molecular Docking and Virtual Screening Software 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 Molecular Docking and Virtual Screening Software market size and forecasts, in consumption value (\$ Million), 2021-2032

Global Molecular Docking and Virtual Screening Software market size and forecasts by region and country, in consumption value (\$ Million), 2021-2032

Global Molecular Docking and Virtual Screening Software market size and forecasts, by Type and by Application, in consumption value (\$ Million), 2021-2032

Global Molecular Docking and Virtual Screening Software market shares of main players, in revenue (\$ Million), 2021-2026

The Primary Objectives in This Report Are:

Global Molecular Docking and Virtual Screening Software Market 2026 by Company, Regions, Type and Application,...

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

To assess the growth potential for Molecular Docking and Virtual Screening Software

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 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.

Market segmentation

Molecular Docking and Virtual Screening Software 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

Structure-Based Docking Software

Ligand-Based Screening Software

Pharmacophore Screening Software

Shape and Electrostatic Similarity Software

AI-Assisted Docking Software

Market segment by Deployment Mode

Desktop Workstation Software

Server or HPC Software

Cloud SaaS Platform

API or Toolkit Software

Hybrid Deployment Software

Market segment by Supported Molecule Type

Small Molecule Docking Software

Fragment Docking Software

Peptide Docking Software

Covalent Ligand Docking Software

Protein-Protein Docking Software

Market segment by License Model

Perpetual License Software

Subscription License Software

Cloud Usage-Based Software

Academic or Free Software

Enterprise Site License Software

Market segment by Application

Hit Discovery

Lead Optimization

Drug Repurposing

Fragment-Based Drug Design

Target Validation and Mechanism Study

Teaching and Academic Research

Market segment by players, this report covers

Schrödinger

Dassault Systèmes

Chemical Computing Group

OpenEye Cadence Molecular Sciences

Cambridge Crystallographic Data Centre

Cresset

BioSolveIT

Molsoft

Molecular Discovery

DP Technology

XtalPi

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 Molecular Docking and Virtual Screening Software product scope, market overview, market estimation caveats and base year.

Chapter 2, to profile the top players of Molecular Docking and Virtual Screening Software, with revenue, gross margin, and global market share of Molecular Docking and Virtual Screening Software from 2021 to 2026.

Chapter 3, the Molecular Docking and Virtual Screening Software 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 Molecular Docking and Virtual Screening Software 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 Molecular Docking and Virtual Screening Software.

Chapter 13, to describe Molecular Docking and Virtual Screening Software research findings and conclusion.

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