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INTEGRATED QSAR, MOLECULAR DOCKING AND MOLECULAR DYNAMICS APPROACHES IN MODERN DRUG DESIGN

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Abstract.

Modern computer-aided drug design increasingly depends on the integration of ligand-based and structure-based methods rather than on the isolated use of a single computational technique. This article presents a structured methodological review of quantitative structure-activity relationship (QSAR) modeling, molecular docking, and molecular dynamics (MD) simulation as complementary components of a contemporary drug-design pipeline. The objective was to analyze how these approaches can be combined to improve hit prioritization, interpret structure-activity relationships, assess binding-mode plausibility, and evaluate the dynamic stability of ligand-target complexes. A focused literature synthesis was performed using fifteen internationally recognized methodological and application-oriented publications covering QSAR best practices, docking algorithms, MD simulation, free-energy estimation, ADMET prediction, and recent integrated case studies. The analysis shows that QSAR is most efficient for rapid activity prediction and chemical-space prioritization, docking provides structural hypotheses for ligand recognition, and MD supplies time-dependent information on conformational adaptation, interaction persistence, solvation, and complex stability. Their sequential and iterative integration reduces method-specific uncertainty and creates a more defensible basis for selecting compounds for synthesis and biological testing. However, predictive value depends strongly on data curation, external validation, applicability-domain assessment, receptor preparation, protonation-state control, force-field quality, simulation convergence, and experimental confirmation. The integrated strategy is therefore best regarded as a decision-support framework rather than a replacement for experimental pharmacology. The review proposes a practical workflow suitable for medicinal chemistry projects and emphasizes reproducibility, transparent validation, and prospective testing as key conditions for scientifically reliable use.

Keywords: quantitative structure-activity relationship; QSAR; molecular docking; molecular dynamics; computer-aided drug design; virtual screening; ADMET; lead optimization.

1. INTRODUCTION

Drug discovery is a multi-stage process in which large numbers of chemical structures are progressively reduced to a small set of candidates with acceptable potency, selectivity, pharmacokinetics, safety, and developability. Because experimental testing of every

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possible chemical structure is impossible, computational methods have become central to early discovery and lead optimization. Among the most established approaches are quantitative structure-activity relationship (QSAR) modeling, molecular docking, and molecular dynamics (MD) simulation. Each method addresses a different layer of the drug-design problem: QSAR connects molecular representation with measured biological response, docking estimates plausible ligand orientations within a binding site, and MD examines how the resulting complex behaves as a dynamic molecular system over time (1,2).

QSAR has evolved from classical linear descriptor models to machine-learning and deep-learning frameworks capable of learning complex nonlinear relationships from molecular fingerprints, physicochemical descriptors, graphs, and learned representations. Despite this methodological expansion, fundamental requirements remain unchanged: chemically meaningful data curation, appropriate endpoint definition, separation of training and external test sets, internal and external validation, and explicit definition of an applicability domain. A statistically impressive model that is trained on inconsistent bioactivity data or used outside its chemical domain may produce misleading predictions (1,2).

Molecular docking provides a structure-based counterpart to ligand-based QSAR. Docking algorithms sample ligand conformations and orientations in a target binding site and rank candidate poses using empirical, knowledge-based, or physics-inspired scoring functions. Programs such as AutoDock Vina have made docking accessible for large virtual-screening campaigns and continue to evolve through improved force-field support, batch processing, flexible-ligand treatment, and scripting interfaces (3,4). However, docking usually treats receptor flexibility only approximately and frequently relies on simplified scoring functions. Consequently, a favorable docking score alone cannot be equated with experimentally confirmed affinity (5,6).

MD simulation addresses several limitations of static docking by propagating the atomic system according to a molecular mechanics force field. It allows investigators to evaluate whether a docked pose remains stable, whether key hydrogen bonds and hydrophobic contacts persist, whether water molecules mediate recognition, and whether the protein undergoes induced-fit or allosteric conformational changes. Modern MD engines can simulate systems containing hundreds of thousands of atoms and provide trajectories suitable for root-mean-square deviation (RMSD), root-mean-square fluctuation (RMSF), hydrogen-bond occupancy, radius-of-gyration, principal-component, and free-energy analyses (7-9).

The central premise of integrated computational drug design is that the weaknesses of one method can be partially compensated by the strengths of another. QSAR can rapidly screen chemical space but may be mechanistically opaque; docking adds spatial interpretation but remains largely static; MD adds dynamics but is computationally more expensive and therefore unsuitable as the first-line filter for millions of molecules. A rational sequence is thus to use QSAR for broad prioritization, docking for structural filtering, and MD for high-resolution validation of a much smaller number of complexes. Recent studies on kinase, bromodomain, metabolic-enzyme, and ion-channel targets demonstrate the growing use of such multi-method strategies (13-15).

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The aim of this article is to systematize the scientific logic, methodological requirements, strengths, limitations, and decision points of an integrated QSAR-docking-MD workflow for modern drug design. Particular attention is paid to validation, reproducibility, ADMET filtering, interpretation of computational outputs, and the boundary between computational evidence and experimentally established pharmacological activity.

2. MATERIALS AND METHODS

This work was designed as a structured methodological review rather than as a report of newly generated biological or simulation data. The evidence base consisted of fifteen internationally cited methodological papers, software papers, reviews, and recent application studies selected to represent the three core components of the integrated workflow: QSAR modeling, molecular docking, and molecular dynamics. Additional emphasis was placed on ADMET prediction and free-energy analysis because these techniques commonly form the bridge between virtual hit identification and lead prioritization.

The literature was synthesized according to four analytical questions: (i) What scientific decision is each computational method intended to support? (ii) What input data and validation procedures are required for reliable use? (iii) Which sources of uncertainty are method-specific? and (iv) How can sequential integration reduce uncertainty before experimental validation? The resulting framework was organized according to an IMRAD structure and summarized in tables and conceptual diagrams. Numerical values shown in the diagrams are qualitative synthesis scales or illustrative decision funnels and are not presented as experimentally measured efficacy data.

2.1. QSAR workflow and validation criteria

A robust QSAR workflow begins with endpoint definition and chemical-data curation. Structures should be standardized with respect to salts, duplicates, valence, aromaticity, tautomerism, stereochemistry, and ionization state. Bioactivity values must represent comparable assay conditions whenever possible. Molecular representation can include constitutional and physicochemical descriptors, 2D fingerprints, topological indices, 3D fields, graph-based features, or learned neural representations. Model selection may range from multiple linear regression and partial least squares to random forests, support-vector machines, gradient boosting, graph neural networks, and deep architectures (1,2).

Validation should combine internal procedures with an independent external test set. Common regression metrics include coefficient of determination (R^2), cross-validated Q^2, root-mean-square error (RMSE), and mean absolute error (MAE), while classification models are commonly evaluated through sensitivity, specificity, balanced accuracy, area under the receiver-operating-characteristic curve, and precision-recall metrics. Y-randomization or response permutation can be used to test whether apparent performance arises from chance correlations. Equally important is the applicability domain, which

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defines the region of chemical space where predictions are considered sufficiently supported by the training data (1).

2.2. Molecular docking protocol

Docking requires careful preparation of both target and ligands. For the receptor, co-crystallized ligands and structurally relevant water molecules should be assessed rather than removed automatically. Missing residues, alternate conformations, metals, cofactors, protonation states, and tautomeric states can materially alter predicted interactions. Ligand preparation includes generation of correct stereochemistry, protonation, tautomers, charges, and low-energy conformations. The docking grid should encompass the biologically relevant binding site defined by a co-crystal ligand, mutagenesis data, known catalytic residues, or validated pocket-prediction methods (3-6).

Protocol validation is essential. Redocking a crystallographic ligand and comparing the predicted and experimental pose by RMSD is a widely used test of whether a specific preparation and parameterization can reproduce the known binding geometry. Enrichment experiments with known actives and decoys provide a stronger assessment for virtual-screening applications. Consensus scoring, visual inspection of chemically plausible contacts, and comparison with established structure-activity relationships can reduce overreliance on a single docking score (5,6).

2.3. Molecular dynamics simulation and trajectory analysis

MD simulations typically proceed through force-field assignment, solvation, ion addition, energy minimization, temperature equilibration, pressure equilibration, and a production trajectory. The simulation length must be adequate for the scientific question and should not be interpreted merely by reaching an arbitrary number of nanoseconds. Convergence, replicate consistency, and stability of relevant observables are more informative than duration alone. Common protein force fields include AMBER and CHARMM families, while ligand parameters may be generated through compatible small-molecule force fields and charge models. GROMACS is one of the widely used high-performance engines for biomolecular MD (7-9).

Trajectory analysis should be hypothesis-driven. Protein backbone and ligand RMSD indicate global positional stability; RMSF identifies flexible residues; hydrogen-bond occupancy and contact-frequency analyses show persistence of interactions; solvent-accessible surface area and radius of gyration describe compactness and exposure; distance and angle monitoring test specific mechanistic hypotheses. Binding free-energy estimates using MM/PBSA or MM/GBSA may assist relative ranking, although their approximations, sampling dependence, and sensitivity to parameterization mean that they should be interpreted comparatively rather than as exact experimental affinities (10).

Table 1. Core roles and validation requirements of the integrated computational methods

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Method	Primary question	Typical output	Key validation requirement	Major limitation
QSAR	Which structures are most likely to show the desired activity?	Predicted activity/probability; feature importance; applicability domain	External test set, cross-validation, Y-randomization, applicability domain	Dependent on training-data quality and chemical-space coverage
Molecular docking	How may a ligand bind in the target site?	Binding poses, scores, interaction map	Redocking, enrichment, structural consistency with known SAR	Static or semi-flexible receptor; imperfect scoring functions
Molecular dynamics	Is the proposed complex dynamically stable and mechanistically plausible?	Trajectory, RMSD/RMSF, contacts, conformational states, free-energy estimates	Equilibration, convergence, replicate consistency, force-field suitability	Higher computational cost and sampling limitations

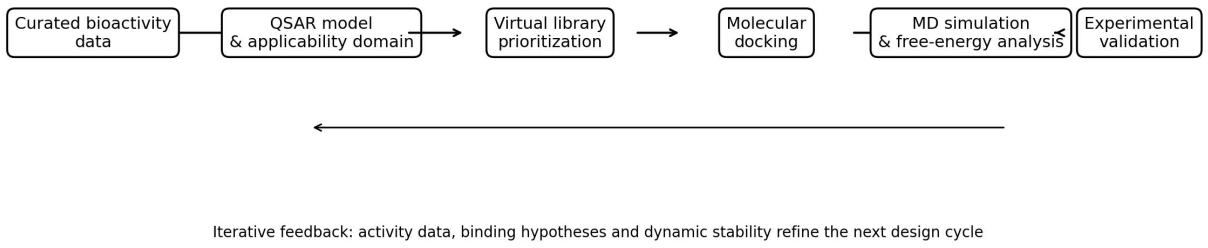


Figure 1. Proposed integrated workflow linking QSAR, docking, MD simulation, and experimental validation.

3. RESULTS

The literature synthesis identified a consistent pattern: QSAR, docking, and MD are most informative when they are treated as complementary decision layers rather than competing prediction methods. Their integration supports progressive reduction of

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chemical space while increasing mechanistic resolution. QSAR operates efficiently at the library level, docking adds target-structure information, and MD concentrates computational resources on a small number of high-priority complexes. This division of labor explains why recent integrated studies frequently use the three methods sequentially rather than independently (13-15).

3.1. QSAR as the first prioritization layer

The principal value of QSAR in an integrated workflow is throughput. Once a model has been validated within a defined domain, it can estimate activity for virtual compounds at negligible marginal computational cost compared with docking or MD. Classical QSAR remains useful for interpretable descriptor relationships, whereas modern machine-learning and deep-QSAR systems can capture nonlinear patterns in large datasets (2). In medicinal chemistry, the most useful QSAR models are not necessarily those with the highest internal R^2; rather, they are those that preserve predictive performance on chemically distinct external compounds and whose uncertainty is explicit.

The review evidence also highlights a second role of QSAR: guiding chemical modification. Descriptor effects, matched molecular pairs, model explanation methods, or learned representations can suggest which molecular properties correlate with potency. These predictions become more actionable when docking is used to determine whether the predicted trend is structurally reasonable. For example, a model may associate hydrophobic substitution with increased activity, while docking can reveal whether the corresponding group occupies a hydrophobic subpocket or instead produces steric conflict. This cross-method consistency is more persuasive than either result in isolation.

3.2. Docking as a mechanistic filter

Docking contributes a structural hypothesis that can discriminate among QSAR-prioritized compounds. The method can identify whether a ligand is geometrically compatible with the binding site, whether key pharmacophoric interactions are possible, and which substituents are oriented toward solvent or unoccupied pockets. AutoDock Vina and related software make this step practical for hundreds to thousands of candidates after an initial ligand-based filter (3,4).

Nevertheless, the literature consistently cautions against interpreting docking scores as direct binding free energies. A difference of one or two scoring units may not correspond to a meaningful experimental difference, especially when compounds differ in size, charge, tautomerism, or flexibility. The strongest use of docking is therefore hypothesis generation and prioritization: candidate poses should agree with known binding-site chemistry, established SAR, and, where available, crystallographic or cryo-EM evidence (5,6).

3.3. MD simulation as a dynamic validation layer

MD provides a test of whether the docked complex remains coherent after relaxation in an explicit dynamic environment. A ligand that rapidly leaves the proposed binding region,

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loses all key contacts, or causes unrealistic structural distortion should be treated cautiously even if its initial docking score is favorable. Conversely, a stable pose that preserves interactions across independent trajectories can strengthen confidence in the structural hypothesis, particularly when the observed contacts explain experimental SAR (7,8).

Dynamic analysis also reveals features that docking cannot capture adequately. Side chains may rotate to accommodate a substituent, loops may open or close, buried water molecules may reorganize, and transient pockets can appear. Such events can alter the interpretation of chemical modifications. In this sense, MD is not merely a "validation after docking" step; it can generate new design hypotheses that feed back into QSAR datasets and the next medicinal-chemistry cycle.

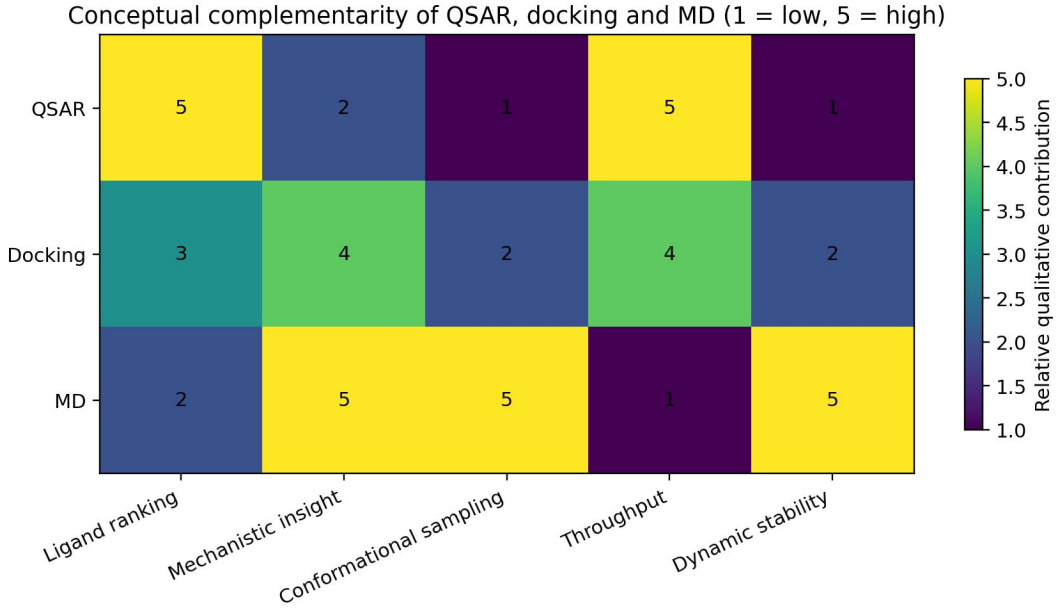


Figure 2. Conceptual comparison of the complementary contributions of QSAR, docking, and MD. The 1-5 scale is qualitative and summarizes methodological roles rather than experimental performance.

Table 2. Recommended quality-control checkpoints in an integrated workflow

Stage	Checkpoint	Acceptable evidence	Common warning sign
Dataset preparation	Chemical and assay curation	Standardized structures; consistent endpoint; duplicate/conflict resolution	Mixed assays or unresolved stereochemistry
QSAR	External predictivity and domain	Independent test performance; stable cross-validation; defined applicability domain	Large train-test gap; randomization test failure
Docking	Protocol validation	Co-crystal redocking	Ranking based only on

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Stage	Checkpoint	Acceptable evidence	Common warning sign
		and/or active-decoy enrichment; plausible interactions	raw score
MD setup	Physical consistency	Appropriate protonation, force field, solvent, ions, equilibration	Unstable temperature/pressure or parameter mismatch
MD analysis	Convergence and reproducibility	Stable observables; repeated trajectories or consistent contact patterns	Single short trajectory used as definitive proof
Lead selection	Orthogonal agreement	QSAR, structural hypothesis, dynamics, ADMET and medicinal chemistry converge	One favorable metric dominates all decisions

4. DISCUSSION

The central advantage of integration is uncertainty reduction through orthogonal evidence. QSAR uncertainty arises primarily from the data and the chemical domain; docking uncertainty arises from sampling, receptor preparation, and scoring; MD uncertainty arises from force fields, initial conditions, and incomplete sampling. Because these uncertainties are different, agreement across methods can increase confidence. Importantly, agreement is meaningful only when each method has been validated independently. Three weak methods do not become strong evidence simply by being combined.

A practical drug-design campaign can therefore be organized as a staged decision funnel. Large chemical collections are first filtered by simple physicochemical rules, undesirable substructures, and validated QSAR models. The smaller set is then subjected to docking against one or more biologically relevant receptor conformations. Compounds are retained not only for favorable scores but also for chemically sensible interactions and diversity. A still smaller set enters MD simulations, where binding-mode stability and dynamic contacts are examined. ADMET models such as SwissADME and pkCSM can be applied throughout the process to prevent potency optimization from producing compounds with obvious developability liabilities (11,12).

Recent integrated application studies support this strategy. Habib and colleagues combined 3D-QSAR, docking, and MD to analyze pyrimidine-based CDK9 inhibitors, showing how ligand-field relationships and structural simulations can be interpreted together (13). Abchir et al. integrated QSAR, docking, ADMET, and MD in the design of triazole derivatives targeting alpha-glucosidase (14). Tong et al. applied QSAR, docking, and MD to the discovery of BRD4-BD2 inhibitors (15). These studies differ in targets and chemical series, but they share the underlying logic of using ligand-based prediction to

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narrow chemical space and structure-based simulation to interpret and refine candidate selection.

The integrated approach is particularly useful when experimental structural information is available. A high-resolution ligand-bound structure can improve docking reliability and facilitate mechanistic interpretation of QSAR trends. When only predicted or homology-modeled structures are available, receptor uncertainty should be explicitly acknowledged and multiple conformations may be required. Ensemble docking followed by MD can partially address receptor flexibility, but it does not eliminate uncertainty in the starting structure.

Another important issue is the relation between docking scores and MD-derived free-energy estimates. Docking is optimized for speed and is appropriate for broad ranking, whereas MM/PBSA or MM/GBSA generally uses trajectory snapshots and a more detailed energetic decomposition. The latter can refine relative ranking within a congeneric series but remains sensitive to conformational sampling, dielectric treatment, entropy approximation, and force-field parameters (10). Free-energy calculations should therefore be interpreted as comparative computational evidence, not as substitutes for experimentally measured Kd, Ki, or IC50 values.

ADMET prediction should not be postponed until the end of the pipeline. A candidate with strong predicted target affinity may still fail because of poor solubility, excessive lipophilicity, metabolic instability, CYP inhibition, hERG liability, or other toxicity risks. SwissADME provides rapid physicochemical, pharmacokinetic, drug-likeness, and medicinal-chemistry assessments, while pkCSM uses graph-based signatures to predict multiple pharmacokinetic and toxicity endpoints (11,12). These predictions are most valuable as early warning systems that guide compound prioritization and experimental planning.

For OAK-oriented scientific reporting and for international publication more generally, reproducibility should be considered a methodological requirement rather than an optional detail. A computational article should report dataset sources and curation rules; descriptor or fingerprint definitions; train-test splitting strategy; random seeds where relevant; software names and versions; docking grid coordinates; scoring settings; protonation assumptions; force fields; water models; ion concentrations; thermostat and barostat choices; equilibration schemes; production length; trajectory sampling frequency; and analysis definitions. Without such information, the work may be difficult to reproduce even if the figures appear convincing.

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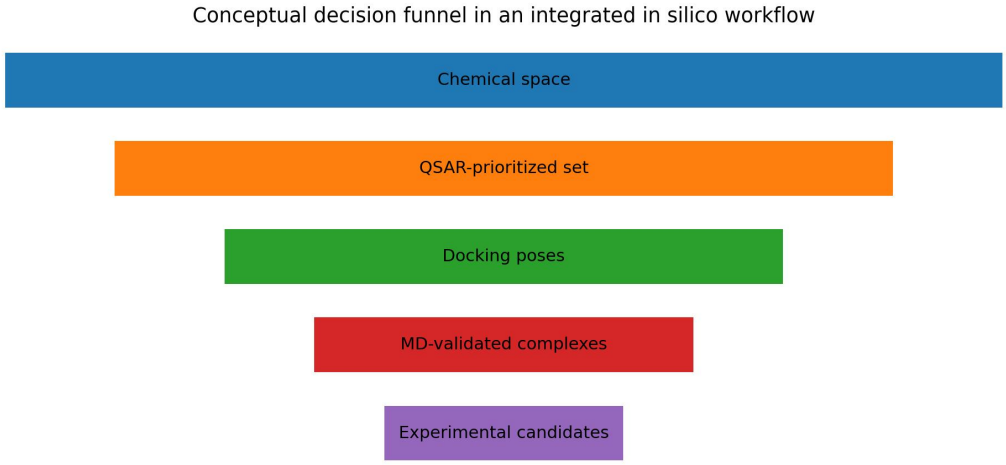


Figure 3. Conceptual decision funnel for integrated virtual screening. Widths are illustrative and do not represent a universal attrition rate.

Table 3. Interpretation of commonly reported computational outputs

Output	What it can support	What it does not prove
High external QSAR performance	Predictive relationship within a defined chemical domain	Mechanism of binding or efficacy in vivo
Favorable docking score	Pose/ranking hypothesis under a specific scoring model	True binding affinity or biological potency
Stable ligand RMSD	Persistence of a particular pose during the simulated time window	Experimental binding or long-term kinetic stability
Persistent H-bond/contact	Possible mechanistic interaction in the modeled complex	That the interaction is essential for activity
Favorable MM/PBSA or MM/GBSA	Relative energetic support within the modeled series	An exact experimental free energy
Favorable ADMET prediction	Lower predicted developability risk	Clinical safety, exposure, or efficacy

A final limitation concerns retrospective confirmation bias. If a computational workflow is developed and tuned on molecules whose biological activities are already known, apparent success may overestimate prospective performance. The strongest evidence comes from prospective prediction: compounds are prioritized before experimental testing, then synthesized or purchased and evaluated in an assay not used to train the model. For this reason, computational integration should culminate in a clearly stated experimental plan rather than in claims that simulation itself has "proved" activity.

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Taken together, the evidence supports a hierarchy of confidence. The lowest level is an unvalidated single-method prediction. Confidence increases when the method is technically validated, when independent computational approaches converge, when predictions remain stable under sensitivity analyses, and finally when the prioritized compound is confirmed experimentally. This hierarchy helps prevent overinterpretation and clarifies the role of in silico methods as scientific decision-support tools.

5. CONCLUSION

Integrated QSAR, molecular docking, and molecular dynamics approaches provide a rational and scalable framework for modern drug design. QSAR is most effective for learning activity patterns from curated chemical data and prioritizing large virtual libraries. Docking adds a structural hypothesis for target recognition and supports interpretation of substituent effects. MD simulation tests these hypotheses under dynamic conditions and can reveal interaction persistence, conformational adaptation, water-mediated effects, and energetically relevant states. ADMET prediction and free-energy analysis further strengthen lead prioritization when applied with appropriate caution.

The scientific value of the integrated workflow does not arise from simply combining software outputs. It arises from validated methods, orthogonal evidence, transparent uncertainty, and iterative feedback between ligand-based and structure-based analyses. Reliable use requires rigorous data curation, external QSAR validation, docking protocol validation, carefully parameterized MD simulations, convergence assessment, and a clearly defined applicability domain. Computational agreement should guide experimental resources toward the most informative candidates, not replace biological testing.

For future drug-discovery projects, the most productive strategy is therefore a prospective and reproducible cycle: curate data, build and validate QSAR models, prioritize diverse compounds, generate and validate binding hypotheses by docking, test dynamic stability by MD, assess ADMET and developability, and finally confirm the predictions experimentally. Such integration can reduce unnecessary synthesis and screening, improve mechanistic understanding, and accelerate the transition from virtual chemical space to experimentally supported lead molecules.

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