



International Journal of Current Trends in Pharmaceutical Research
 Home Page: <https://pharmaresearchlibrary.org/journals/index.php/ijctpr>
 CODEN (USA): IJCTGM | ISSN: 2321-3760 | Publisher: Pharma Research Library
 Int. J. Curnt. Tren. Pharm, Res., 2025, 13(2): 90-96
 DOI: <https://doi.org/10.30904/j.ijctpr.2025.4865>



A Review of SwissADME in Morden Medicinal Chemistry: Insights on Anti-Cancer, Anti-Tubercular, and Anti-Microbial Agents

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ABSTRACT

The process of drug discovery has evolved dramatically with the integration of computational tools capable of predicting key pharmacokinetic and physicochemical parameters of small molecules. SwissADME, a freely available web-based tool developed by the Swiss Institute of Bioinformatics, provides medicinal chemists with an efficient platform to assess parameters such as lipophilicity, solubility, bioavailability, and drug-likeness. This review presents a comprehensive overview of the applications of SwissADME in the design and development of anticancer, antitubercular, and antimicrobial agents. The study emphasizes the importance of *in silico* ADME predictions in lead optimization, compound prioritization, and rational drug design. Furthermore, it discusses how SwissADME complements molecular docking, QSAR, and pharmacophore modeling in streamlining preclinical research. Comparative insights with other ADME tools, including pkCSM and admetSAR, are also provided. The review concludes with current limitations and future directions, highlighting the integration of SwissADME with artificial intelligence and machine learning for improved predictive accuracy in drug discovery.

Keywords: SwissADME, ADME prediction, Drug-likeness, Pharmacokinetics, Anticancer agents

ARTICLE INFO

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Article History:

Received 05 Aug 2025
 Revised 31 Aug 2025
 Accepted 29 Sep 2025
 Published 09 Oct 2025

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Citation: Shaik Mohammad Rafi, *et al.* A Review of SwissADME in Morden Medicinal Chemistry: Insights on Anti-Cancer, Anti-Tubercular, and Anti-Microbial Agents. Int. J. Curnt. Tren. Pharm, Res., 2025, 13(2): 90-96.

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1. Introduction

In recent years, *in silico* methods have fundamentally transformed the landscape of small molecule drug discovery. By integrating computational approaches such as hit identification, lead optimization, binding free energy and interaction pattern analysis, dynamic simulation, and critically the prediction of physicochemical and pharmacokinetic (ADMET) properties, researchers

dramatically accelerate and refine the drug development process. These computational jobs, previously time-consuming in wet-lab settings, are now efficiently handled using a variety of user-friendly platforms.(1) Among the available tools, SwissADME stands out due to its free accessibility, intuitive interface, and robust suite of predictive algorithms. It allows medicinal chemists to

quickly evaluate vital molecular properties spanning lipophilicity, solubility, size, polarity, pharmacokinetics, and drug-likeness filters. Additional modules provide deep insights into drug-likeness, flagging problematic substructures (like PAINS) and visualizing results through features like the BOILED-Egg and Bioavailability Radar thereby aiding both the selection and optimization of lead compounds at early research stages. By providing rapid feedback and actionable data, SwissADME empowers medicinal chemists to make informed, evidence-driven choices throughout the drug development cycle. As a freely accessible, reliable, and comprehensive computational tool, it effectively bridges high-throughput *in silico* screening with traditional experimental workflows, helping researchers focus resources on the most promising candidates across oncology, tuberculosis, and infectious disease domains. This collective review underlines SwissADME's pivotal contribution as a cornerstone technology in modern small-molecule drug discovery and offers practical guidance for its optimal use in ongoing and future medicinal chemistry research. (2)

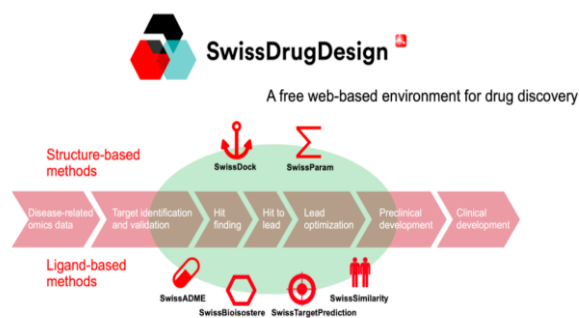


Fig.1: Swiss Drug Design

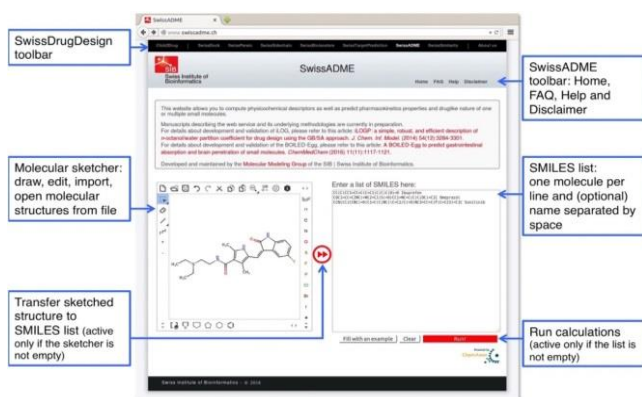


Fig.2: User interface of ADME

2. Procedure for using SwissADME Predictions for A Dataset of Compounds: SwissADME allows batch evaluation of multiple compounds for ADME (Absorption, Distribution, Metabolism, and Excretion), drug-likeness, and physicochemical properties. Below is a structured procedure for performing SwissADME predictions using a dataset of compounds.

2.1 Prepare Your Dataset

Obtain or design your compounds: You can gather molecules from sources like PubChem(3), ChemSpider (4), or design new structures using molecular editors such

as MarvinSketch (5) or ChemDraw (6). Should contain one compound per line with the following format: in text for example CC(=O)Oc1ccccc1C(=O)O Aspirin, CCC(=O)NCCO Penicillin. Convert each molecule to SMILES format: Prepare an input text file: Each line We can enter up to 200 molecules at once as recommended by SwissADME.

2.2 Access the SwissADME Web Server

Open your browser and go to the official website: www.swissadme.ch. (7) On the homepage, you'll see a text box labeled SMILES list this is where you'll input your dataset.

2.3 Input Your Compounds

There are two main ways to input your dataset:

Option A: Paste SMILES manually Copy your SMILES list and paste it directly into the input field in swissadme.ch.

Option B: Use the Molecular Sketcher Click "Molecular Sketcher (Marvin JS)" to draw or import molecular structures. Click the double arrow (\Rightarrow) to generate the SMILES, then press Add to list. Repeat for multiple compounds.

2.4 Run the Prediction

Once your list of compounds is entered, button the Run

1. on the interface will turn red.
2. Click Run. The computation starts (typically 1–5 seconds per drug-like molecule).

2.5 Interpret the Output

After computation, SwissADME displays results directly below the input box.

Main Output Sections:

Physicochemical Properties: Reports molecular weight, number of rotatable bonds, hydrogen bond donors/acceptors, molar refractivity, and TPSA.

- **Lipophilicity:** Displays logP values estimated by five models — iLOGP, XLOGP3, WLOGP, MLOGP, and SILICOS-IT — alongside a consensus logP value.
- **Water Solubility:** Predicts logS using methods like ESOL and Ali to indicate solubility class.
- **Pharmacokinetics:** Predicts GI absorption, BBB crossing, P-gp substrate behavior, and potential CYP450 inhibition.
- **Drug-likeness Filters:** Applies Lipinski, Ghose, Veber, Egan, and Muegge rules to assess oral drug suitability.
- **Medicinal Chemistry Alerts:** Identifies PAINS, Brenk alerts, and synthetic accessibility score (scale 1–10).
- **Bioavailability Radar:** A hexagonal (radar) visualization mapping lipophilicity, size, polarity, solubility, flexibility, and saturation.
- **BOILED-Egg Plot:** Graphical prediction showing likelihood of GI absorption and brain access.

2.6 Export or Save the Results Main Output Sections:

Alternatively, copy the results into Excel or another spreadsheet for further analysis.

2.7 Analysing and Using Results

Cross-compare key metrics like consensus logP, TPSA, solubility (logS), and synthetic accessibility to prioritize compounds. Apply drug-likeness filters to quickly identify suitable lead scaffolds. Assess pharmacokinetic parameters to select compounds with optimal balance between lipophilicity, solubility, and oral absorption.

Correlate ADME data with docking or in vitro results for better structure-activity relationship (SAR) interpretation.

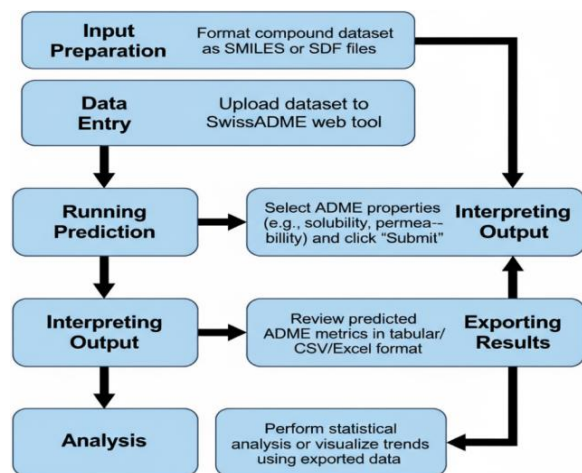


Fig.3: Flow chart for Using SwissADME Predictions

3. Core Functional Modules of SwissADME

SwissADME integrates multiple in-house and validated predictive models, allowing users to assess a molecule's Absorption, Distribution, Metabolism, and Excretion (ADME) behavior with high accuracy. This approach helps researchers understand how changes in chemical structure may influence bioavailability, solubility, permeability, and metabolic stability in human systems.

3.1 Physicochemical Property Predictions

SwissADME calculates essential parameters such as molecular weight, topological polar surface area (TPSA), hydrogen bond donors and acceptors, rotatable bonds, molar refractivity, and molecular saturation. These values help predict solubility, membrane permeability, and target accessibility properties critical for both oral and injectable drugs.

3.2 Lipophilicity Estimators

It employs multiple models such as iLOGP, XLOGP3, WLOGP, MLOGP, and SILICOS-IT to estimate logP, (8) a measure of lipophilicity. Since lipophilicity impacts a molecule's absorption, membrane passage, and bioavailability, comparing results across models provides a robust insight into pharmacokinetic performance.

3.3 Water Solubility Models: Swiss ADME predicts a molecule's aqueous solubility using models like ESOL, Ali, and SILICOS-IT. Accurate solubility estimation across different pH levels helps in formulation development and determining a compound's suitability for oral or parenteral administration.

3.4 Pharmacokinetic Simulations

A central module of SwissADME predicts ADME-related factors, including gastrointestinal absorption, blood-brain barrier permeability, P-glycoprotein substrate recognition, and CYP450 enzyme inhibition potential. These descriptors are essential for assessing oral bioavailability and drug-drug interaction risks.

3.5 Drug-Likeness Filters

SwissADME automatically evaluates a compound's compliance with established drug-likeness rules, such as the Lipinski Rule of Five, Ghose (9), Veber (10), Egan (11), and Muegge filters (12). These rules define

boundaries for molecular weight, lipophilicity, hydrogen bonding potential, and polarity, helping to gauge a compound's likelihood of oral activity.

3.6 Medicinal Chemistry Friendliness Alerts

The tool flags the presence of Pan-Assay Interference Compounds (PAINS) (13), Brenk structural alerts, and reactive functional groups, which may cause assay artifacts or instability. It also computes a Synthetic Accessibility (SA) Score that estimates synthetic feasibility based on fragment frequency and structural complexity (14).

3.7 The Bioavailability Radar

This unique graphical visualization simplifies the assessment of a compound's overall "drug-likeness." It displays six parameters — lipophilicity, size, polarity, solubility, flexibility, and saturation — over a radar chart, where values inside the pink area represent the optimal range for oral bioavailability (15).

3.8 The BOILED-Egg Model

The Brain Or Intestinal Estimated permeation method (BOILED-Egg) is a simple, visual classifier that predicts whether a molecule is likely to be absorbed passively via the gastrointestinal tract or capable of crossing the blood-brain barrier. Compounds appearing inside specific zones of the "egg" diagram indicate desirable pharmacokinetic profiles.



Fig.4: BOILED-Egg Model

4. Importance in Medicinal Chemistry

SwissADME bridges the gap between computational prediction and experimental drug design. Its integrated modules allow researchers to:

- Rapidly screen chemical libraries for promising leads
- Visualize ADME-related trade-offs between solubility, lipophilicity, and permeability,
- Optimize molecules for pharmacokinetic balance early in the pipeline
- Minimize late-stage attrition by predicting problematic properties.

5. SwissADME Applications in Drug Design

5.1 Antiproliferative Activity Applications

Rotenone analogues were studied by a group of researchers in 2024 to explore their possible antiproliferative and cytotoxic effects against various human cancer cell lines such as MCF-7 (breast), A549 (lung), and HCT116 (colon). The study involved in silico evaluation of the

designed derivatives using the SwissADME web tool to predict their physicochemical and pharmacokinetic parameters. Swiss ADME predicted acceptable oral absorption, drug-likeness, and solubility profiles for most derivatives. It was also observed that these analogues complied well with Lipinski's Rule of Five, confirming their potential for oral bioavailability. Furthermore, the analysis through Bioavailability Radar and BOILED-Egg models showed high gastrointestinal absorption capacity. This study confirmed that SwissADME is an effective tool for early-stage screening of natural product-based anticancer leads, providing reliable predictions for the molecular optimization process(16).

Another significant investigation was carried out by Mohamed Sheik Tharik and Meyyanathan (2023) to establish correlations between *in vitro* and *in vivo* pharmacokinetic behaviors of several anticancer kinase inhibitors, namely Axitinib, Ibrutinib, Icotinib, Nilotinib, and Dasatinib. The study utilized SwissADME to predict solubility, lipophilicity, and bioavailability and to compare the computational results with experimental data. The predictions showed high digestive absorption and balanced lipophilicity values within the therapeutic window, validating SwissADME's high accuracy in ADME profiling. The authors concluded that the software's features like the physicochemical and consensus logP value and Bioavailability Radar enable researchers to visually interpret critical pharmacokinetic parameters prior to *in vivo* experimentation, thus making it a valuable method for data-driven drug optimization(17).

In 2024, another computational study focused on curcumin analogues, well known for their anticancer potential but limited by low bioavailability and metabolic instability. The modified curcumin compounds were analyzed using SwissADME and DFT (Density Functional Theory) to evaluate the physicochemical and ADME properties. The program predicted improved solubility, lower polarity, and enhanced gastrointestinal absorption for methylated and hydrogenated derivatives. The BOILED-Egg diagram suggested that some analogues might cross the blood-brain barrier (BBB), potentially increasing systemic efficacy. The combined SwissADME and DFT data confirmed that altering functional how platform SwissADME serves as a convenient and predictive for screening and improving herbal analogues with potential anticancer activity(18).

In 2020, SwissADME was applied in a pharmacokinetic evaluation study involving novel synthetic anticancer scaffolds to identify promising candidates with optimal drug-likeness. The compounds' molecular descriptors such as molecular weight, topological polar surface area (TPSA), hydrogen-bond donor/acceptor capacity, and lipophilicity—were predicted through the SwissADME pipeline. All the screened candidates followed Lipinski's, Veber, and Ghose rules, suggesting a high probability of oral bioavailability. The tool was also used to eliminate compounds that exhibited poor solubility or high flexibility. The researchers concluded that SwissADME's

rapid, rule-based screening approach minimized time and cost in drug design, thereby increasing the reliability of early-stage anticancer lead generation(19).

A study conducted in 2023 on oxindole derivatives combined SwissADME, DFT, and docking analyses to characterize newly synthesized compounds. These molecules were screened for their *in silico* ADME profiles using SwissADME, where all major variants passed common drug-likeness filters such as Lipinski, Ghose, and Muegge rules. Predictions indicated good GI absorption, suitable logP, and acceptable synthetic accessibility scores. These computational evaluations indicated enhanced pharmacological compatibility and reduced metabolic risk. The study concluded that coupling SwissADME's predictions with quantum chemical calculations improved the accuracy of pharmacokinetic predictions and expedited the lead selection process for new oxindole-derived anticancer drugs(20).

5.2 Role in Antitubercular Drug Development

Tuberculosis persists as a major challenge due to pathogen resilience and drug resistance. The nature of *Mycobacterium tuberculosis*—the complex cell wall, persistence, and intracellular survival—demands agents that not only have potent activity but also optimal ADME attributes.

Screening and Filtering: SwissADME quickly evaluates scaffold libraries for antitubercular potential, focusing on parameters linked to cell wall penetration, oral bioavailability, and metabolic fate.

ADME with SAR: Investigations into compounds such as ethambutol and benzimidazole analogues linked predicted ADME properties with Structure-Activity Relationships (SAR), identifying substitution patterns (e.g., electron-withdrawing groups) that favor permeability and systemic distribution. A research team in 2025 investigated a collection of 1,2-disubstituted benzimidazole derivatives for their potential as antitubercular agents using a combination of molecular docking and *in silico* pharmacokinetic assessment. SwissADME and related tools were employed to predict each compound's ADME properties, focusing particularly on drug-likeness and oral bioavailability. The results revealed that most of the designed benzimidazole derivatives not only complied with key drug-likeness filters but also showed favorable pharmacokinetic profiles, including good gastrointestinal absorption and acceptable solubility. The computational experiments supported these findings, with lead compound P32 demonstrating a stronger binding affinity for the FtsZ protein target of *Mycobacterium tuberculosis* than some standard TB drugs. The authors emphasized that while the SwissADME predictions are promising for prioritization, further *in vitro* and *in vivo* validation is necessary to confirm biological activity(21).

Another recent investigation, published in 2022, focused on the widely used anti-tubercular drug ethambutol to compare SwissADME's predictive validity with experimental pharmacokinetic data. By inputting ethambutol's molecular structure into the SwissADME platform, researchers generated predictions on its

absorption, bioavailability, and target profile. These predicted parameters mostly mirrored those observed in experimental and clinical reports, with the tool accurately suggesting moderate oral absorption and active distribution. In addition to validating its current use, the study highlighted SwissADME's capacity to inform the re-design or reformulation of established drugs, as well as to aid in the prediction of other potential anti-tubercular agents before undertaking synthesis or animal studies (22). Researchers in 2024 synthesized several β -aminopropioamidoxime derivatives and tested their antitubercular efficacy against both drug-sensitive and multidrug-resistant strains of *Mycobacterium tuberculosis*. SwissADME was used as a central tool to evaluate these molecules' drug-likeness, lead-likeness, gastrointestinal absorption, and synthetic accessibility. The compounds passed most major ADME criteria, suggesting that they are promising scaffolds for further optimization. Importantly, the study demonstrated how in silico filtering with SwissADME assists researchers in narrowing down hit lists to molecules most likely to succeed in subsequent in vitro and in vivo efficacy tests, especially when targeting resistant mycobacterial infections (23).

5.3 Antimicrobial Multi-Target Screening

In 2023, a research group designed a series of quinoline derivatives with potential antibacterial activity against multi-drug resistant bacterial strains. The study employed SwissADME to predict physicochemical parameters such as lipophilicity, solubility, and topological polar surface area (TPSA), alongside pharmacokinetic properties including gastrointestinal absorption and blood-brain barrier (BBB) permeability. Following the in silico SwissADME analysis, all compounds passed Lipinski's and Veber's rules, showing promising drug-likeness and oral bioavailability. The results guided compound prioritization before synthesis, with lead analogues demonstrating better predicted absorbance and membrane permeability profiles. The combined computational and antibacterial testing validated SwissADME's role in expediting antimicrobial agent development(24). Another study conducted in 2022 focused on the antimicrobial potential of natural-product-based benzimidazole scaffolds. The researchers utilized SwissADME to predict various ADME parameters including solubility, absorption, and cytochrome P450 enzyme inhibition potential. Compounds with favorable SwissADME profiles showed high potential for oral administration and low toxicity risk. Subsequent biological assays confirmed robust activity against Gram-positive and Gram-negative bacteria. The study highlighted SwissADME as an integral tool for guiding the optimization of natural product derivatives targeting resistant microbes, enabling a balance between efficacy and favorable pharmacokinetics(25).

A 2024 investigation synthesized several imidazole-based compounds to assess antifungal activity. SwissADME was used to evaluate drug-likeness, gastrointestinal absorption, and synthetic accessibility of these molecules. The in silico predictions revealed that most compounds had good predicted oral bioavailability and moderate water solubility, with acceptable synthetic feasibility scores,

supporting their practical development. Antifungal assays demonstrated potent activity against *Candida* species, aligning with the drug-likeness features projected by SwissADME. The study concluded that SwissADME provides crucial preliminary data that optimize compound libraries for antifungal drug discovery efficiently(26).

6. Future Directions

The field of computational drug discovery continues to evolve, and SwissADME is expected to keep pace through several emerging trends:

Artificial Intelligence Integration: Machine learning models using larger and more diverse datasets may improve property prediction for complex molecules and novel chemical space (27).

Customized Predictive Modules: Development of disease- or target-specific property predictors could extend SwissADME's applicability, such as tailoring models for blood-brain barrier prediction or special metabolic pathways in pathogens(28).

Expanded Interoperability: Further integration with virtual screening, molecular dynamics, and toxicology platforms will create robust multi-parametric pipelines for medicinal chemists(29).

Community-Curated Datasets: Incorporation of user feedback and real experimental outcomes into training datasets will refine predictive algorithms and improve reliability (30).

SwissADME is poised to remain at the forefront of computational filtering and optimization in early-phase drug discovery.

7. Conclusion

Swiss ADME fundamentally shifts the paradigm of drug discovery by streamlining the design, prioritization, and advancement of small-molecule therapeutics. Its user-friendly web interface, comprehensive predictive suite, and efficient batch analysis capabilities have made it an essential tool for medicinal chemists working on anticancer, antitubercular, and antimicrobial agents (31). While its predictions must be balanced with empirical evidence and consideration of outlier cases, Swiss ADME greatly accelerates rational drug design, resource allocation, and candidate selection. As computational models, data science, and artificial intelligence develop further, the role of tools like SwissADME will only grow, bringing more precision and efficiency to the pipeline of therapeutic innovation.

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