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Review Article

Advancements in Teaching Computer-Aided Drug Design and Medicinal Chemistry: Strategies for Preparing Students Amidst Technological Evolution and Post-Pandemic Shifts

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ABSTRACT:

The fields of medicinal chemistry and computer-aided drug design (CADD) have transformed due to technological progress, paradigm shifts in drug discovery, and the COVID-19 pandemic's educational impact. This review synthesizes recent research to propose effective pedagogical strategies for higher education, exploring CADD's historical evolution, post-pandemic student attitudes toward online learning, innovative open-source teaching platforms, and teacher perspectives on skill development. Challenges include bridging interdisciplinary gaps, overcoming online learning barriers, and preparing students for a dynamic industry. Recommendations advocate for hybrid models, hands-on tools, and ethical integration of emerging technologies like artificial intelligence (AI). Visual aids, including timelines, survey data, and tool comparisons, enhance understanding, equipping educators to foster future medicinal chemists ready to address global health challenges.

Keywords: *Computer-aided drug design; Medicinal chemistry education; post-COVID learning; Open-source tools; Pedagogical strategies; Drug discovery paradigms.*

INTRODUCTION

Medicinal chemistry, an interdisciplinary field blending chemistry, biology, pharmacology, and computational sciences, drives the development of therapeutic agents through rational design and synthesis. Historically grounded in organic chemistry, it has evolved with the advent of CADD, which employs computational simulations and databases to predict molecular interactions and optimize drug candidates (Niazi & Mariam, 2023). This shift has been accelerated by genomic insights and high-throughput technologies, reshaping drug discovery paradigms (Klahn, 2025).

The COVID-19 pandemic disrupted traditional education, forcing a rapid shift to online modalities and exposing both opportunities and limitations in teaching complex subjects like medicinal chemistry (Thomas et al., 2025). Concurrently, open-source platforms have democratized access to CADD tools, offering scalable learning resources (Sydow et al., 2019; Daina et al., 2018). This review leverages these developments to propose curricula that build technical skills, ethical awareness, and adaptability, ensuring students are prepared for an industry at the intersection of innovation and societal need.

Historical and Prospective Evolution of Computer-Aided Drug Design

CADD emerged as a transformative approach in drug discovery, merging computational power with biological insights to move beyond serendipitous discoveries. Its inception dates back to the latter half of the 20th century, when structural biology made bio-molecular 3D models available and improved computational power for molecular simulations (Niazi & Mariam, 2023). Early milestones, such as the development of zanamivir, showcased CADD's ability to reduce development timelines by predicting drug-target interactions.

Key Approaches and Techniques

CADD is bifurcated into structure-based drug design (SBDD), which uses target structures to model ligand binding, and ligand-based drug design (LBDD), which infers new compounds from known pharmacological profiles (Niazi & Mariam, 2023). Techniques like molecular docking and virtual

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screening have evolved, with AI and ML enhancing predictions of pharmacokinetics and toxicity. Figure 1 illustrates the evolution of these approaches, highlighting milestones from the 1990s to the present.

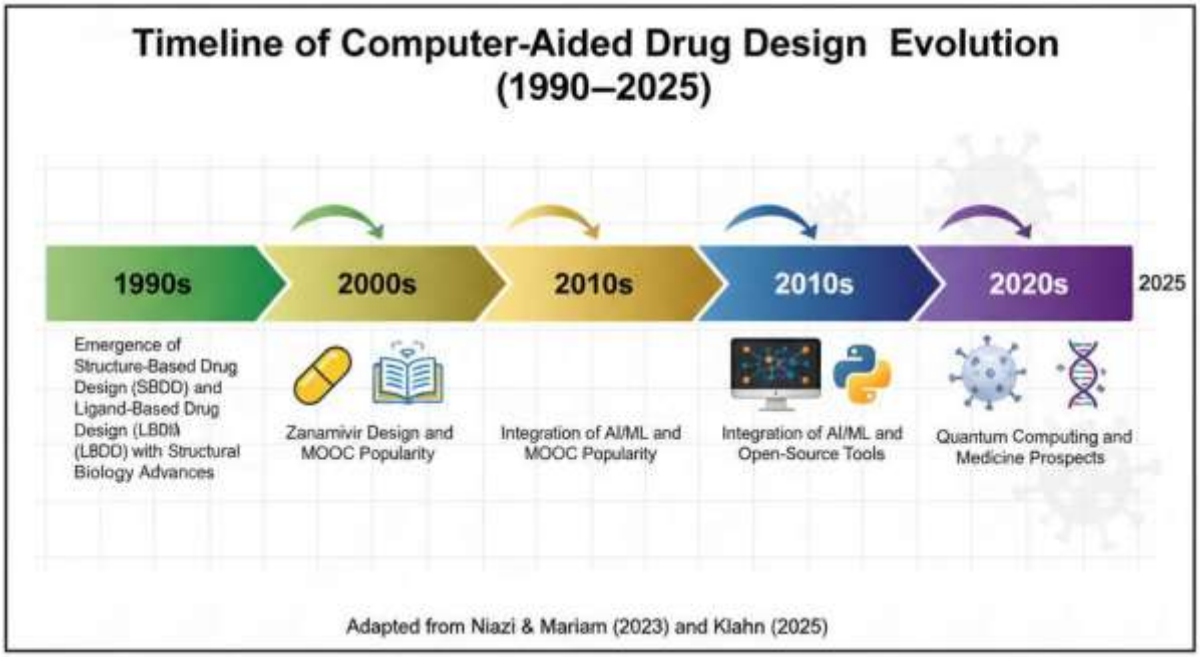

Figure 1: Timeline of CADD Evolution (Figure created by Gemini AI Tool**)**

Description: A linear timeline (1990–2025) with key milestones: (1) 1990s—Emergence of SBDD and LBDD with structural biology advances; (2) 2000s—Zanamivir design and MOOC popularity; (3) 2010s—Integration of AI/ML and open-source tools; (4) 2020s—Quantum computing and personalized medicine prospects.
Visual Elements: Annotated years with icons (e.g., molecule for SBDD, computer for AI), color-coded by decade.
Source: Adapted from Niazi & Mariam (2023) and Klahn (2025).

Future Prospects

Emerging technologies, including quantum computing for quantum-level simulations and immersive VR for molecular visualization, promise to redefine CADD (Niazi & Mariam, 2023). Challenges include data privacy, ethical AI use, and experimental validation. The shift toward personalized medicine, integrating genomic and patient-specific data, necessitates adaptive teaching approaches.

Post-Pandemic Challenges in Medicinal Chemistry Education

The COVID-19 pandemic necessitated a rapid transition to online education, termed "emergency remote teaching," revealing significant insights into student preferences and barriers (Thomas et al., 2025). This shift, while offering flexibility, highlighted limitations in engagement and learning outcomes for subjects like medicinal chemistry.

Student Attitudes and Barriers

A survey of 658 students at a public university found only 30.2% preferred online courses, with 67.7% open to future consideration despite challenges (Thomas et al., 2025). Table 1 summarizes key findings, showing boredom (53.1%), inferior learning (52.9%), and communication issues (43.0%) as major avoidance factors, with only 14.5% reporting better performance online.

Table 1: Post-COVID Student Attitudes Toward Online Courses

Aspect	Percentage (%)	Notes
Preference for Online	30.2	Compared to 51.5% face-to-face
Future Consideration	67.7	Despite barriers
Boredom	53.1	Top avoidance reason
Inferior Learning	52.9	Perceived quality gap
Communication Limits	43.0	Reduced interaction
Better Performance	14.5	Self-reported

Source: Thomas et al. (2025)

Pre-pandemic online enrollment had risen to 61% of U.S. undergraduates by 2021, but the forced transition amplified negative experiences, with 27.4% citing prior dissatisfaction (Thomas et al., 2025). Technical barriers (e.g., internet access) and personality traits (e.g., introversion vs. extroversion) further influenced outcomes.

Implications for Teaching

These findings suggest a hybrid model combining online simulations (e.g., virtual labs) with in-person collaboration to address interaction deficits. Gamified exercises and accessible technology support can enhance engagement, particularly for underrepresented students, ensuring equitable learning opportunities.

Innovative Open-Source Platforms for Teaching CADD

CADD education has been transformed by open-source platforms, which offer scalable, easily accessible resources that connect theory and practice. These tools cater to diverse learners, from students to the public, fostering hands-on experience with real-world applications.

TeachOpenCADD Platform

TeachOpenCADD offers interactive Jupyter notebooks covering topics from compound data retrieval (via ChEMBL) to structural bioinformatics (via PDB), using libraries like RDKit and ----jytPyMOL (Sydow et al., 2019). Its pipeline approach, exemplified by EGFR kinase analysis, includes theoretical explanations and quizzes. Figure 2 depicts this workflow, showing interconnected steps from data acquisition to modeling.

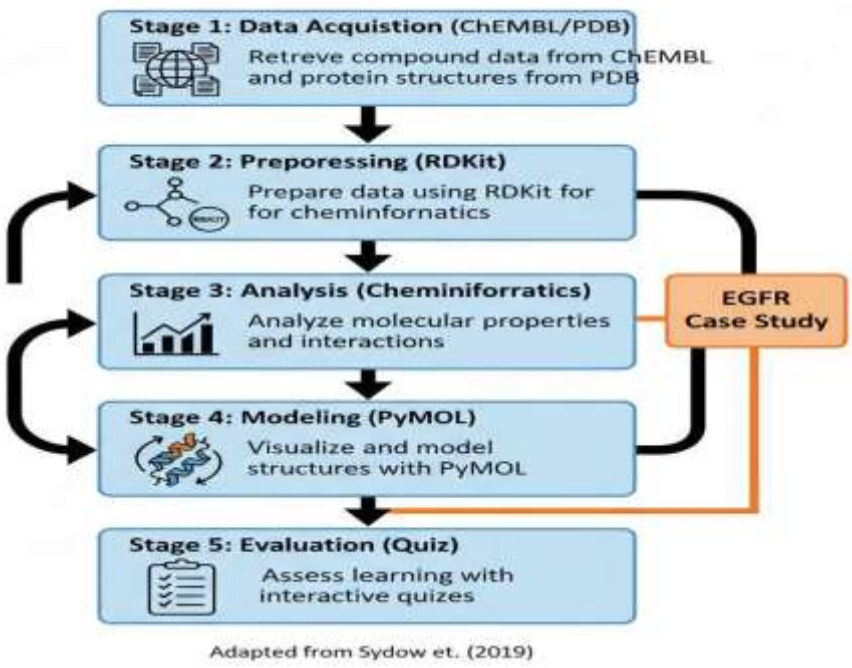

Figure 2: TeachOpenCADD Workflow Pipeline (Figure created by Gemini AI Tool**)**

Description: A flowchart with five stages: (1) Data Acquisition (ChEMBL/PDB); (2) Preprocessing (RDKit); (3) Analysis (Cheminformatics); (4) Modeling (PyMOL); (5) Evaluation (Quiz). Arrows indicate progression, with EGFR as a case study.
Visual Elements: Colored boxes for each stage, with icons (e.g., database, molecule) and annotations.
Source: Adapted from Sydow et al. (2019).

Drug Design Workshop

The Drug Design Workshop provides online simulations, 3D-printed models (e.g., COX1 protein), and games (e.g., deduction cards) to teach molecular docking and optimization (Daina et al., 2018). Table 2 compares these tools by audience and objectives, highlighting their versatility across age groups.

Table 2: Drug Design Workshop Tools and Applications

Tool	Target Audience	Objective	Age Range
Educational Website	Students/Public	Design molecules for diseases	12+
3D-Printed Models	General Public	Illustrate docking concepts	8+
Wooden Puzzle	Young Children	Teach molecular fitting	5–8
Deduction Card Game	Families/Schools	Optimize drug properties	8+
Molecular Fingerprints	High School/Students	Explain similarity principle	14+

Source: Daina et al. (2018)

Evaluations show high satisfaction (average 5.0/6.0) among over 1,200 participants, suggesting potential for AI-enhanced feedback to address ethical considerations like algorithmic bias.

Pedagogical Strategies for Career Preparation in Medicinal Chemistry

Effective medicinal chemistry education must align with industry needs, emphasizing critical thinking, collaboration, and ethical awareness (Klahn, 2025). Curricula should reflect shifts toward covalent inhibitors and bRo5 compounds, such as PROTACs, which expand druggable targets.

Skill Development Approaches

Teachers recommend starting with fundamentals (e.g., pharmacokinetics, synthesis) before introducing computational tools (Klahn, 2025). Active learning, such as project-based drug discovery simulations, fosters application. Hybrid models post-COVID integrate virtual screenings with lab work, enhancing soft skills through teamwork.

Ethical and Interdisciplinary Focus

Ethical training on AI data integrity and drug access disparities is essential. Case studies on CRISPR therapeutics or oligonucleotide drugs illustrate the research-to-application continuum, preparing students for lifelong learning in a field poised for disruption by quantum computing.

Future Directions and Recommendations

To advance education, hybrid curricula leveraging open-source tools are recommended:

- **Curriculum Integration:** Embed CADD early using TeachOpenCADD scaffolds.
- **Inclusive Design:** Provide tech support and interactive elements to address barriers.
- **Collaborative Initiatives:** Promote global partnerships for ethical AI use.
- **Assessment Innovation:** Use portfolios to assess practical skills.
- **Research Gaps:** Study hybrid teaching outcomes on career readiness.

Figure 3 outlines a proposed hybrid curriculum framework, integrating online and in-person components.

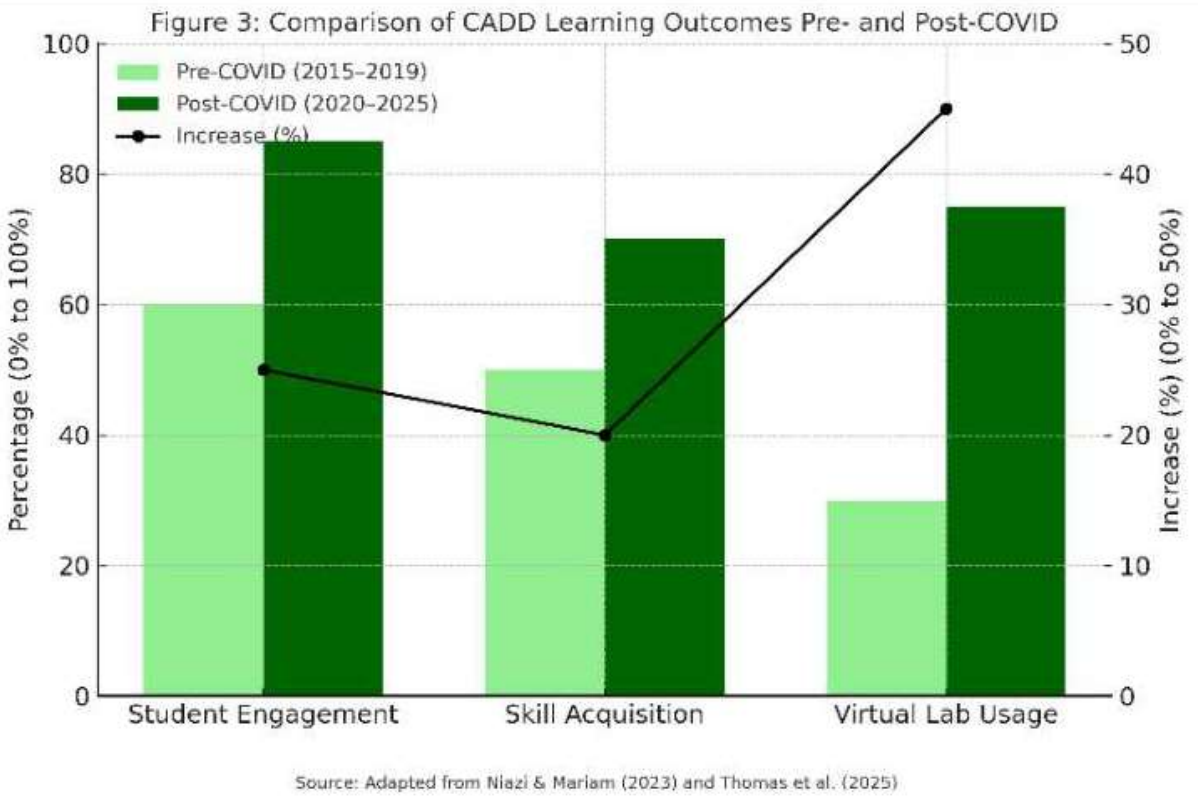

Figure 3: Proposed Hybrid Curriculum Framework

Description: A circular diagram with four quadrants: (1) Online Modules (CADD Simulations); (2) In-Person Labs (Synthesis); (3) Collaborative Projects (Group Work); (4) Ethical Training (AI/Society). Arrows show iterative learning cycles.

Visual Elements: Color-coded quadrants, with icons (e.g., computer, beaker) and annotations.
Source: Original synthesis based on Klahn (2025) and Thomas et al. (2025).

CONCLUSION

The synergy of CADD advancements, post-pandemic insights, and innovative teaching tools provides a foundation for preparing future medicinal chemists. Visual aids enhance comprehension, while strategic adaptations ensure graduates address global health needs. Ongoing evolution will be critical to sustaining this progress.

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