

Integrating BioSolveIT in Health Professions Curricula: Bridging Academia and Industry

Alaa J.Mahrath ¹ , Samar Hasan Shammar ² , Zaenab Mohsen Najm ³

Abstract

The rapid advancements in pharmaceutical research and development demand a systematic transformation in pharmacy education to align academic training with industry needs. In this research, we explore the integration of BioSolveIT's computational tools, such as the SeeSAR software program, into pharmacy curricula as a means to bridge the gap between academia and modern pharmaceutical industries. BioSolveIT's innovative software enables drug discovery processes like molecular docking, ligand-based drug design (LBDD), and fragment-based lead discovery, which have become increasingly important in contemporary pharmaceutical discoveries. Despite their widespread use in industry, these tools remain underutilized in pharmacy education, leaving graduates unprepared for roles requiring computational expertise. By incorporating BioSolveIT into coursework, our students gain hands-on experience with cutting-edge technologies, enhancing their understanding of molecular interactions and drug optimization. Therefore, this study highlights the benefits of integrating computational tools into pharmacy education, including improved student competency, alignment with industry trends, and enhanced career readiness. However, challenges such as limited faculty training, curriculum time constraints, and resource availability must be addressed to ensure successful implementation. An analysis of pharmacy curricula across the country's governorates confirms the necessity for pharmacy programs to adopt integrated curricula based on cases that combine basic pharmaceutical sciences with practical applications of modern tools. In conclusion, this research highlights the transformative potential of BioSolveIT in equipping future pharmacists with the skills needed to succeed in the evolving pharmaceutical landscape, drive innovation, and meet healthcare demands nationally and globally.

Keywords: Healthcare Curricula, BiosolveIT, Molecular Modeling, learning outcomes

دمج تطبيقات BioSolveIT في مناهج المهن الصحية: ربط الأوساط الأكاديمية بالصناعة

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المستخلص

يتطلب التطور السريع في البحث والتطوير الدوائي تحولاً منهجياً في تعليم الصيدلة لمواءمة التدريب الأكاديمي مع احتياجات الصناعة. في هذا البحث، نستكشف دمج أدوات BioSolveIT الحاسوبية، مثل برنامج SeeSAR، في مناهج الصيدلة كوسيلة لسد الفجوة بين الأوساط الأكاديمية والصناعات الدوائية الحديثة. يُمكن برنامج BioSolveIT المبتكر عمليات اكتشاف الأدوية، مثل الالتحام الجزيئي، وتصميم الأدوية القائمة على الرابطة (LBDD)، واكتشاف الرصاص الجزأ، والتي أصبحت ذات أهمية متزايدة في الاكتشافات الدوائية المعاصرة. على الرغم من استخدامهما على نطاق واسع في الصناعة، إلا أن هذه الأدوات لا تزال غير مستغلة بشكل كافٍ في تعليم الصيدلة، مما يجعل الخريجين غير مؤهلين للأدوار التي تتطلب خبرة حاسوبية. من خلال دمج BioSolveIT في المقررات الدراسية، يكتسب طلابنا خبرة عملية في التقنيات المتطورة، مما يعزز فهمهم للتفاعلات الجزيئية وتحسين الأدوية. لذلك، تُسلط هذه الدراسة الضوء على فوائد دمج الأدوات الحاسوبية في تعليم الصيدلة، بما في ذلك تحسين كفاءة الطلاب، ومواكبة اتجاهات الصناعة، وتعزيز الجاهزية المهنية. ومع ذلك، لا بد من معالجة تحديات مثل محدودية تدريب أعضاء هيئة

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معلومات البحث

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التدريس، وضيق الوقت المخصص للمناهج الدراسية، وتوافر الموارد لضمان نجاح التنفيذ. ويؤكد تحليل مناهج الصيدلة في جميع محافظات البلاد ضرورة اعتماد برامج الصيدلة مناهج متكاملة قائمة على دراسات حالة تجمع بين العلوم الصيدلانية الأساسية والتطبيقات العملية للأدوات الحديثة. وفي الختام، يُسلط هذا البحث الضوء على الإمكانيات التحويلية لـ BioSolveIT في تزويد صيادلة المستقبل بالمهارات اللازمة للنجاح في المشهد الدوائي المتطور، ودفع عجلة الابتكار، وتلبية متطلبات الرعاية الصحية على الصعيدين الوطني والعالمي.

الكلمات المفتاحية: مناهج الرعاية الصحية، BiosolveIT، النمذجة الجزيئية، نتائج التعلم

1. Introduction

Rapid technological advancements have revolutionized the healthcare sector, transforming the way healthcare workers are trained and prepared to perform their duties professionally[1]. In an era where accuracy, efficiency, and adaptability are paramount, computational software has emerged as indispensable tools in the education and development of healthcare workers[2]. These programs not only bridge the gap between theoretical knowledge and practical application, but also provide students with essential skills that enhance their problem-solving abilities, decision-making processes, and professional competence [3]. For pharmacy students, biologists, and other healthcare learners, computational tools such as BioSolveIT provide a dynamic platform for simulating realistic scenarios, analyzing complex biological systems, and designing innovative solutions [4].

These computational programs have gained a particularly valuable place in healthcare curricula, enabling students to interact with cutting-edge technologies that meet the demands of modern healthcare environments. For example, SeeSAR 12.1, a molecular modeling and drug discovery tool, enables pharmacy students to visualize molecular interactions, predict drug efficacy, and optimize therapeutic compounds [5]. This hands-on experience fosters a deeper understanding of

pharmacological principles and prepares students to contribute effectively to drug development and patient care. Similarly, biology students benefit from computational tools by gaining insights into genomic data analysis, protein folding, and systems biology, which are essential for the development of personalized medicine and biotechnological innovations [6].

Numerous studies have highlighted the role of computational programming tools in healthcare education. According to a study published in the Journal of Medical Education, integrating simulation-based learning into medical and pharmaceutical curricula significantly improves students' clinical reasoning and technical skills [7]. Similarly, a report published in Drug Discovery highlights how computational platforms accelerate drug discovery processes, enabling students to understand the complexities of molecular interactions and drug design [8]. These findings underscore the need to integrate computational software into healthcare education to ensure students are well prepared for the challenges of the future healthcare landscape.

Moreover, computational tools enhance interdisciplinary collaboration, a cornerstone of modern healthcare practice [9]. By introducing students to shared platforms and methodologies, these programs bridge the gaps between disciplines, such as pharmacy, biology, medicine,

and bioinformatics. This collaborative approach provides a clear and integrated picture of the delivery of appropriate healthcare and promotes a comprehensive understanding of patient care [10].

The computer programs, such as SeeSAR 12.1, play a pivotal role in shaping the future of healthcare education. They empower students with advanced skills, encourage innovation, and prepare them to meet the evolving demands of the healthcare sector [11]. As healthcare systems

around the world continue to embrace digital transformation, integrating computer tools into curricula is not just an option, but a necessity for building competent, forward-thinking healthcare professionals [12]. Therefore, it was important to develop our educational curricula based on modern software supported by artificial intelligence technologies to open new horizons for developing health professions curricula. as shown in Figure (1).

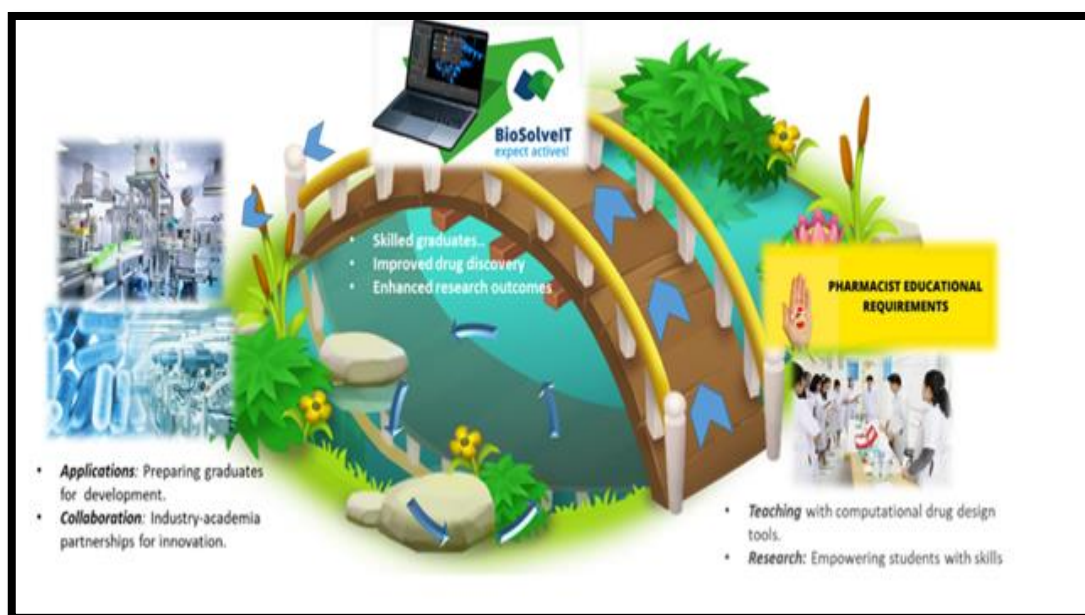


Figure (1): Integrating BioSolveIT in Pharmacy Curricula: Bridging Academia and Industry

Hence, this research paper came to demonstrate the mechanisms for using such modern software in school curricula.

2. Materials and Methods [13]

The materials required include licensed software, high-performance hardware, curated datasets, and classroom infrastructure. The methodology involves defining objectives, integrating SeeSAR into the curriculum, training users, and evaluating outcomes. as follows:

2.1: Materials Required:

1. Software

SeeSAR 12.1: Ensure licensed access to the software for all students and faculty. BioSolveIT offers academic licenses for educational institutions.

Supporting Tools: Additional software such as molecular databases (e.g., Research Collaboratory for Structural Bioinformatics (RCSB) [14], Protein Data Bank (PDB), PubChem[15], and visualization tools like, PyMOL[16], Chimera[17].

2. Hardware

- a) **Computers:** High-performance computers or laptops with sufficient specifications to run SeeSAR smoothly:
- b) **Processor:** Intel Core i5/i7 or equivalent.
- c) **RAM:** Minimum 8 GB (16 GB recommended).
- d) **Graphics Card:** Dedicated GPU for better rendering of molecular structures.
- e) **Storage:** At least 10 GB free space for installation and datasets.
- f) **Network Infrastructure:** Reliable internet connection for accessing online resources and databases.

3. Educational Resources

- a) **Datasets:** Curated datasets of proteins,

ligands, and drug targets for practice and projects.

- b) **Tutorials and Manuals:** Step-by-step guides and instructional videos for using SeeSAR.
- c) **Case Studies:** Real-world examples of drug discovery projects to illustrate practical applications.

4. Classroom Setup

- a) **Computer Lab:** A dedicated lab equipped with the necessary hardware and software for practical sessions.
- b) **Interactive Tools:** Projectors or smartboards for demonstrating software features during lectures.
- c) **Implementation Examples.** as shown in Figure (2).

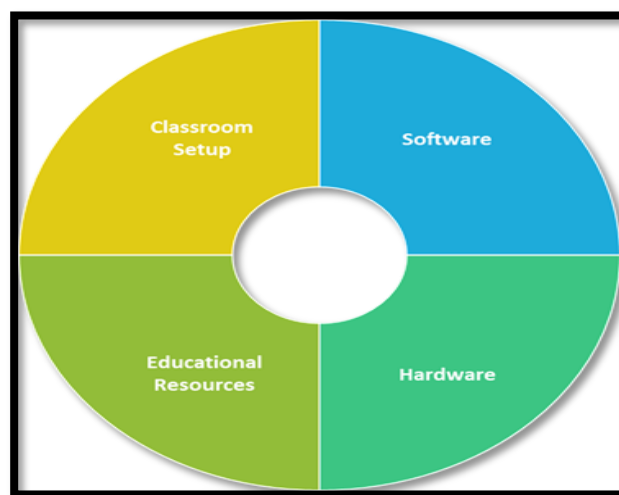


Figure (2): Comprehensive Educational Setup for SeeSAR

2.2. Method

Module: Drug Design and Discovery

Week 1: Introduction to Molecular Modeling:

Lecture: Overview of molecular docking and its importance in drug discovery.

Practical: Basic navigation and visualization in SeeSAR.

Week 2: Ligand-Receptor Interactions:

Lecture: Principles of ligand binding and affinity prediction.

Practical: Docking experiments using SeeSAR.

Week 3: Optimization of Drug Candidates

Lecture: Strategies for improving drug efficacy and safety.

Practical: Use SeeSAR to modify molecular structures and evaluate changes in binding affinity.

Week 4: Group Project

Students work in teams to design a drug candidate

targeting a specific protein.

Present findings using SeeSAR-generated visualizations. as shown in Figure (3).

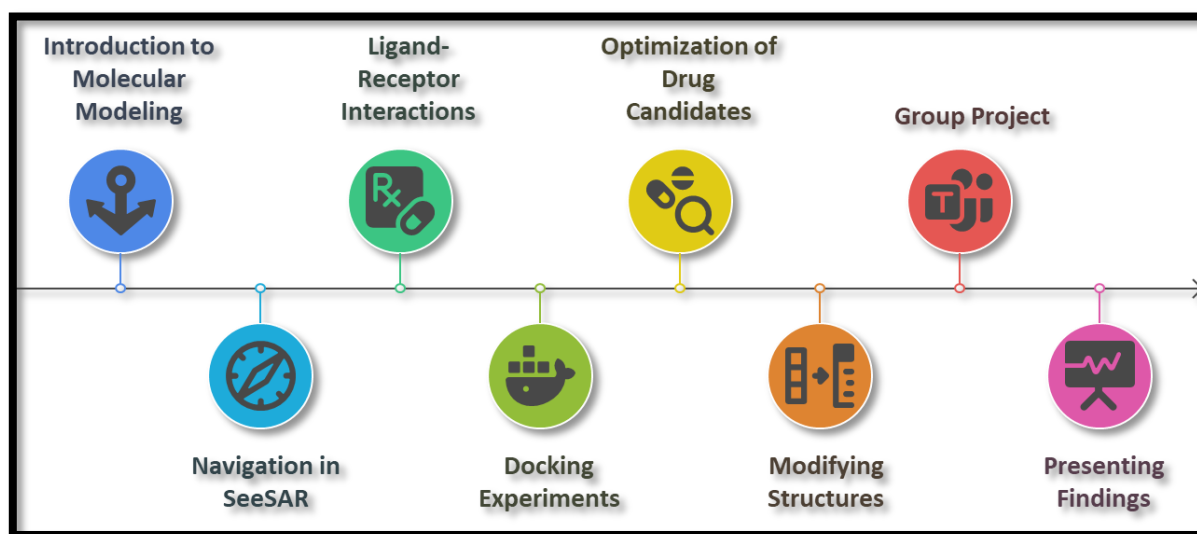


Figure (3): Drug Design and Discovery Module Sequence

Methodology

1. Define Objectives and Learning Outcomes

The first step is to clearly define the objectives of integrating SeeSAR 12.1 into the medical curriculum. These objectives should align with the broader goals of the program, such as:

- Enhancing students' understanding of molecular interactions and drug design.
- Teaching computational methods for drug discovery and optimization.
- Bridging the gap between theoretical knowledge (e.g., biochemistry, pharmacology) and practical applications in drug development.

Learning Outcomes:

Students will be able to visualize and analyze molecular structures and interactions.

Also, they will learn to use computational tools to predict drug-target interactions.

And will develop critical thinking skills by designing and optimizing hypothetical drug molecules.

2. Curriculum Integration Plan

Integrate SeeSAR 12.1 into specific modules or courses within the medical curriculum. Examples include:

- Pharmacology Courses: Introduce SeeSAR as a tool for understanding drug-receptor interactions.
- Biochemistry Courses: Use it to explore enzyme inhibition mechanisms and ligand binding.
- Research Methodology Courses: Teach computational drug discovery techniques and data analysis.

Integration Steps:

Lecture Component: Provide theoretical

background on molecular modeling, docking, and drug design.

Practical Sessions: Hands-on training with SeeSAR 12.1 to reinforce concepts.

Project-Based Learning: Assign projects where students use SeeSAR to solve real-world problems, such as designing a molecule to target a specific disease-related protein.

3. Training Faculty and Students

Before implementing SeeSAR 12.1, ensure that both faculty and students are adequately trained:

Faculty Training: Conduct workshops or training sessions for instructors to familiarize them with the

software's features and capabilities.

Student Training: Provide step-by-step tutorials and hands-on practice sessions for students.

4. Evaluation and Feedback

Evaluate the effectiveness of SeeSAR integration through:

Assessments: Include assignments, quizzes, and exams that require students to use SeeSAR to solve problems.

Feedback Surveys: Collect feedback from students and faculty to identify challenges and areas for improvement. as shown in Figure (4).

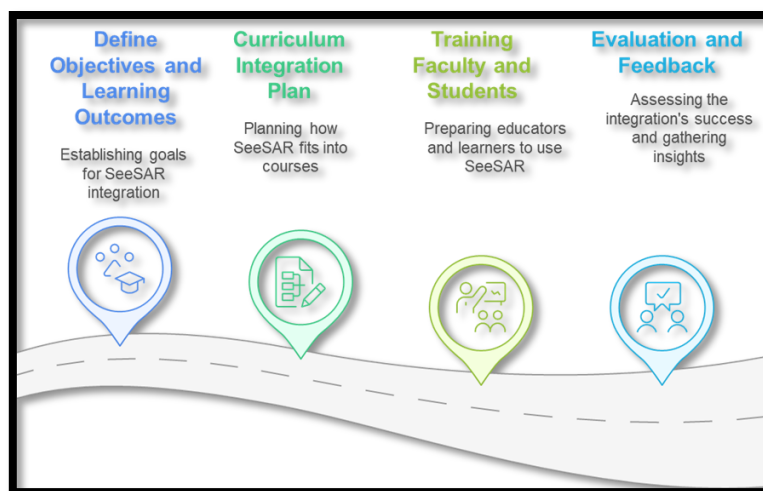


Figure (4): Integrating SeeSAR 12.1 into Medical Curriculum

3. Results and Discussion:

Through the experiences of scientifically advanced countries, the integration of BioSolveIT tools, particularly SeeSAR 12.1, into healthcare curricula has shown promising results in enhancing the learning experience and bridging the gap between theoretical knowledge and practical applications in drug discovery and molecular design[18]. Therefore, our findings were:

Enhanced Understanding of Molecular Interactions: Students demonstrated a deeper understanding of molecular docking, ligand-

receptor interactions, and drug-target binding mechanisms. Also, visualizations provided by SeeSAR helped simplify complex concepts, making them more accessible to learners.

Improved Practical Skills in Drug Design:

Training with BioSolveIT tools equipped students with practical skills in computational drug discovery, such as virtual screening, lead optimization, and affinity prediction. Also, students were able to design and evaluate hypothetical drug molecules, fostering creativity and problem-

solving abilities.

Bridging Theory and Practice:

The use of BioSolveIT tools allowed students to apply theoretical knowledge from pharmacology, biochemistry, and medicinal chemistry to real-world scenarios. Case studies and project-based learning further reinforced the connection between academic concepts and industry practices.

Increased Engagement and Motivation:

Interactive and visually engaging software like SeeSAR increased student engagement and motivation.

The gamified nature of designing and optimizing molecules made learning enjoyable and less complicated [19].

Preparation for Modern Healthcare Challenges:

Graduates exposed to BioSolveIT tools were better prepared for careers in pharmaceutical research,

personalized medicine, and other cutting-edge fields.

The curriculum aligned with industry trends, ensuring that students acquired skills relevant to current and future healthcare demands[20].

Positive Feedback from Faculty and Students:

Both faculty and students reported high satisfaction with the integration of BioSolveIT tools.

Faculty appreciated the ease of teaching complex topics with visual aids, while students valued the hands-on experience and real-world applicability [21].

By reviewing the results, we find the following:

The successful integration of BioSolveIT tools into healthcare curricula highlights their potential to transform traditional teaching methods. By incorporating computational tools like SeeSAR, teachers can create a dynamic and interactive learning environment that addresses the limitations of purely theoretical instruction. as shown in Figure (5).

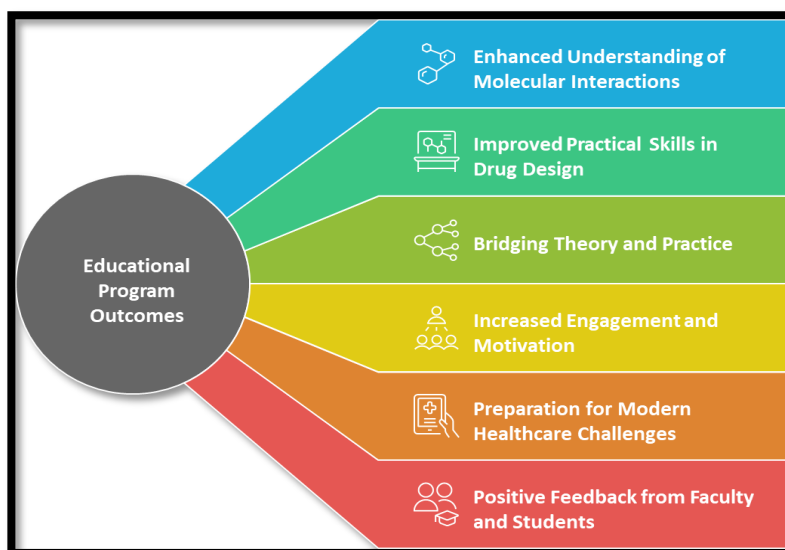


Figure (5): the Multifaceted Impact of Education

Also, BioSolveIT tools provide a user-friendly interface and powerful visualization capabilities, making advanced concepts accessible even to

beginners. The emphasis on practical skills ensures that students are not only knowledgeable but also capable of applying their learning in professional

settings.

However, main Challenges, are the Initial costs for software licensing and hardware upgrades may pose financial challenges for some institutions. Faculty require adequate training to effectively teach and troubleshoot the software, which may demand additional time and resources.

Conclusion

The use of BioSolveIT tools in healthcare curricula has yielded significant educational benefits, including improved conceptual understanding, enhanced practical skills, and increased student engagement. While some challenges remain, the overall impact highlights the importance of embracing innovative technologies in medical education. By equipping students with the tools and skills necessary for modern healthcare, institutions can ensure that graduates are prepared to meet future challenges in drug discovery and patient care.

Recommendation: as healthcare increasingly relies on computational tools and precision medicine, integrating platforms like BioSolveIT into curricula prepares students for the evolving landscape of medical research and practice. Expanding access to such tools across institutions could expand education in drug discovery and related fields.

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