Transforming Academic Research:
A Business Model for
Chemical-Computational Laboratory

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Abstract – **The Business Model Canvas (BMC) is a transformative tool in business strategy, streamlining the creation of dynamic models for organizational success. In the evolving field of academic research, computational chemistry undergoes significant changes due to increased computational capabilities and algorithm refinement. Despite these advancements, the challenge remains in effectively translating computational insights into commercial outcomes. This study addresses the task of formulating a business model for a computational simulation research lab and integrating a strategic Strengths-Weaknesses-Opportunities-Threats (SWOT) analysis. Also, to identify predominant trends within computational chemistry research articles through literature review and keyword frequency analysis. A nine-block business model for a computational chemistry research lab was crafted using the BMC template. SWOT analysis was applied to each block of the business model. Trends in computational chemistry appear to be in drug discovery, following material design. Business model designing, meticulous market analysis like literature review trends, and strategic planning doing SWOT analysis are essential pillars supporting the successful execution of research projects.**

1. Introduction

In the dynamic and changing global landscape, enterprises spanning diverse sectors are incessantly engaged in the quest for inventive strategies that will ensure their competitiveness and pertinence. Among these sectors, the chemical industry is a pivotal cornerstone of modern civilization. Nonetheless, this industry confronts formidable obstacles in its pursuit of expansion and durability in a sustainable way. In this context, the advent of digitalization emerges as an indispensable instrument for fostering the advancement of sustainable practices [1].

Computational chemistry has undergone a paradigm shift fueled by exponential growth in computational capabilities and refined algorithms. This transformation has significantly altered the landscape of drug discovery [2]. Yet, a persistent obstacle lies in effectively translating computational insights into tangible commercial outcomes. To overcome this challenge, the Business Model Canvas (BMC) [3] presents a structured framework that holds the potential to bridge this gap. By facilitating research labs in delineating precise objectives and aligning research resources, the BMC offers a strategic avenue for progress. At the core of this effort lies the convergence of business strategy, comprehensive internal-external analyses, and the execution of scientific projects – encapsulated within the conceptualization of a business model for a Computational Simulation Research Lab (CSRL). This business model not only streamlines research endeavors but also emerges as a potent instrument to harmonize the aspirations of CSRLs with the dynamic demands of the industry. As such, the CSRL business model is a pivotal step toward harnessing the untapped potential of computational chemistry and its seamless integration into drug development and commercialization.

The BMC, a strategic management instrument, visually depicts a comprehensive business model. It encompasses nine fundamental building blocks: customer segments, value propositions, channels, customer relationships, revenue streams, key activities, key resources, key partners, and cost structure [3]. This framework has garnered widespread adoption as a versatile tool for strategic analysis [4], conceptualization [5], and evolution of business models [6]. Exploring these blocks enables CSRLs to craft an all-encompassing overview of its operations, illuminating areas primed for enhancement and refinement.

On the other hand, CSRL stands at the vanguard of computational chemistry, embodying a field where scientists employ advanced algorithms [7], [8], [9] in conjunction with simulations to anticipate and enhance molecular properties [10], reactions [11], and sophisticated processes [12]. This revolutionary methodology not only propels the accuracy of predictions but also expedites the optimization of these properties. By employing this innovative approach, CSRLs impart remarkable efficiencies to research and development endeavors [13], ushering in a paradigm shift in the traditional workflow. This approach substantially curtails the demand for resource-intensive experimental testing [14], [15], leading to a more streamlined and sustainable research process.

The amalgamation of BMC and CSRL presents an opportunity for research and innovation. By integrating the BMC's strategic insights, capabilities of CSRL, and market research, organizations can unlock new dimensions of innovation and drive sustainable growth [16], [17], [18]. This integration allows organizations and enterprises to make data-driven decisions, optimize product portfolios, streamline production processes, and continuous innovation [19]. For example, Self-Driving Labs (SDLs) utilize data science to automate experimentation, integrating machine learning, lab automation, and robotics [14].

This research gives scientists, researchers, and project managers an intricate comprehension of the adept adaptation and effective utilization of the BMC. By harmonizing the inherent scientific objectives with business strategies and data-driven market research, the BMC emerges as a formidable instrument that empowers scientific practitioners to navigate the intricate commercialization landscape deftly. Moreover, this strategic alignment aids in securing vital funding and amplifying the societal reverberations of their scientific undertakings. Through the lens of an applied case study accompanied by pragmatic insights, this paper takes on the role of inspiration, illuminating the diverse advantages, obstacles, and reflections that come to the front while implementing the BMC within research labs.

At its center, this research aspires to catalyze a transformative shift conducting wherein scientific innovation seamlessly intertwines with the ability of intelligent business expertise. This integration not only cultivates a fertile ground for entrepreneurship but also propels a wave of change within the scientific community, setting a new era of harmonious convergence between scientific skill and business expertise. This study successfully developed a targeted business model for a computational simulation research lab, accompanied by a thorough strategic SWOT analysis. This study asserted the pivotal role of meticulous planning, market analysis, and strategic design in achieving successful research project execution.

2. Methodology

The business model for a computational simulation research laboratory (CSRL) was designed using the Osterwalder methodology. Strategic insights into the business model's strengths, weaknesses, opportunities, and threats were gained through a SWOT analysis. In addition, the study employed a combination of qualitative and quantitative research methodologies for analyzing secondary data.

2.1. Business Model Canvas

The business model was designed utilizing Osterwalder methodology without changes [3]. Nine blocks were analyzed for a CSRL localized in Santiago de Chile. Strategic analysis was made to identify the business model's strengths, weaknesses, opportunities, and threats using SWOT analysis according to the methodology described [20], [21].

2.2. Secondary data

Qualitative and quantitative research methodology was used to analyze data. Four criteria were established to search key trends on Scopus databases using the ScienceDirect search engine, according to Table 1. Each keyword detailed in Criteria I and II was searched according to Criteria III and IV. The number of annually published research articles for each keyword was registered. The average annual growing rate of publications for each keyword was calculated yearly according to Equation 1. The average annual growth rate was calculated for four periods of time, (1990-1999), (2000-2009), (2010-2019) and (2020-2022).

$$Equation\ 1: \left(\frac{present - past}{past}\right) * 100$$

Table 1. Criteria keyword search details

Criteria	Detail
I	**Principal areas** mathematics physics chemistry biology
II	**Computational chemistry** database simulation algorithm computational data analysis computational material design computational molecular modeling computational chemical reaction computational drug discovery
III	Research article type
IV	From years 1990 to 2022

3. Results and Discussion

The BMC for a CSRL was designed, as shown in Figure 1. The first block is *Customer segments (CS)*, which are critical to understanding the needs and building customer-oriented companies [22]. The customer segment identified for the CSRL was academic researchers. Researchers in computational and other research areas are potential collaborators to work on paper publications or write grant proposals. The second block is the *Value proposition (VP)*, which describes the benefits and value of products and services offered to specific *CS*. This concept was influential in the chain value analysis that helps identify the source of value creation [23].

The *VP* identified for researchers is to increase research productivity. Researchers face pressure to publish and increase the chance to grant funds for research [24]. For example, the three principal aims in the academic medical field are education, discovery, and the use of knowledge to improve patient care [25]. In the research field, publishing increases knowledge and understanding of specific areas. The third block is *Channels (CH)*, which are very important to communicate the *VP* to a particular *CS*. Having different *CH* increases the chance of delivering communicational campaigns [26]. The CSRL has two *CH*, online platforms, and a physical lab. The fourth block is *Customer relationships (CR)*, the relationship between the company and a specific customer segment. The purpose of *CR* for the CSRL was personal assistance, where online platforms or presential meetings directly connected researchers. The fifth block is *Revenue streams (RS)*, the flux of benefits from specific customer segments. In this case, the CSRL received benefits from the *CS*, *Key partners (KP)*, and Governmental funding. The *CS* provided collaboration, the *KP* gave infrastructure to install the simulation lab, and the National Agency of Research and Development (ANID) granted funds for research. Infrastructure sponsorship and publications are crucial to applying for government funding. The sixth block is *Key resources (KR)*, the most essential resource to execute the *VP*. For the CSRL computers, the Internet, researchers, and funds are the key resources. Simulation computers support experiments or tests. The Internet is essential for database and remote working. Researchers are individuals who write grant proposals and have the knowledge to execute experiments.
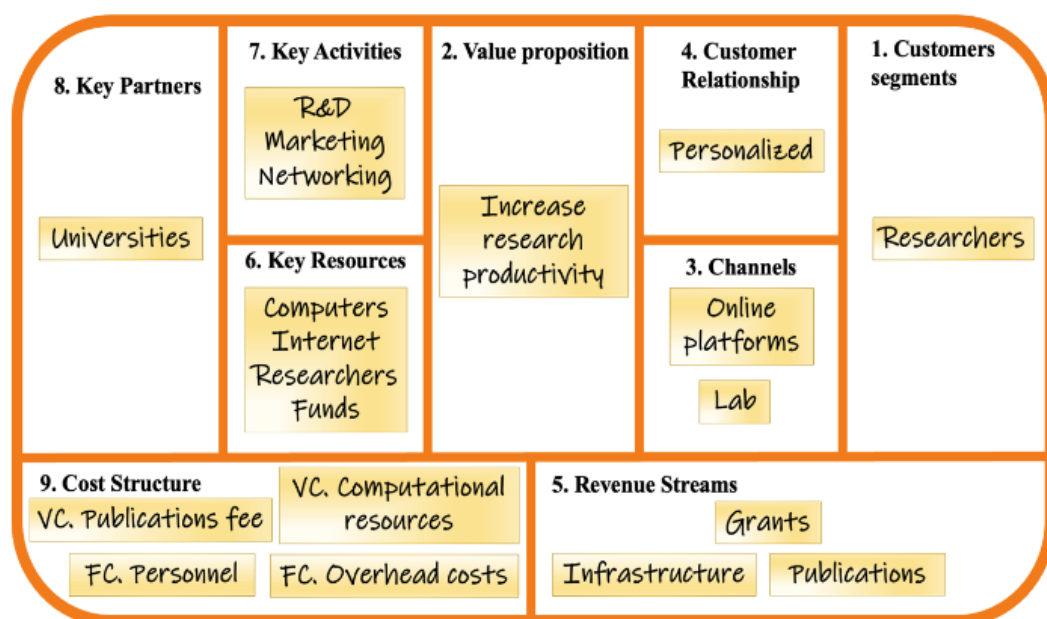

Figure 1. Business model canvas for a computational research lab

Funds are vital to any research project. The seventh block is *Key activities (KA)*, the most critical to achieving the value proposition. Research and development (R&D), marketing, and networking are essential for a CSRL. R&D aims to improve existing services, products, and processes or create innovations. Marketing is critical to communicating research findings and capabilities. Networking is essential to growing the collaboration between researchers from different fields [28], [27]. The eighth block is *Key Partners (KP)*, suppliers, or partners necessary to execute the *VP*. A healthy partnership is based on balanced trust and control [29], [30]. The *KP* for the CSRL is a private university that allowed research on its buildings. This partnership is essential for grant proposals requirement. The ninth and last block is *Cost structure (CSE)*, which implies all the efforts of the company to execute the value proposition. There are variable costs (VC) and fixed costs (FC). For the CSRL overhead costs, the researcher, technician, and student salary are FC. Computer resources for experiments increase depending on the investigations. VC relates to computational resources for experimental testing that may increase with demand, like the computer software program Gaussian 16.

Creating a comprehensive and strategic BMC personalized for the unique requirements of a cutting-edge research lab emerges as an indispensable instrument, wielding formidable prowess in the seamless execution of research projects. This meticulously crafted BMC serves as a facilitator and appears as an adept diagnostic apparatus, illuminating the multifaceted landscape of the lab's capabilities. By meticulously dissecting each canvas component, the lab gains a nuanced comprehension of its strengths, which serve as the bedrock for future advancements while equally unearthing its vulnerabilities. This incisive introspection propels a relentless pursuit of refinement, fostering an environment where weaknesses evolve into opportunities. Additionally, this strategic blueprint empowers the lab to orchestrate its resource allocation with surgical precision, channeling them into avenues that promise optimal yield. In research projects, where precision and efficiency reign supreme, the art of designing a personalized BMC stands as a facilitator of projects and a vanguard of transformative progress.

Then, a Strengths, Weaknesses, Opportunities, and Threats (SWOT) analysis was applied, identifying one variable for each business model block, as shown in Figure 2. The strength of the CSRL for *CS* was simulation knowledge, which is important to guide other researchers, students, and potential investors.

The power of the *VP* has been validated by the experience of the principal investigator by publishing in peer-reviewed journals [31], [32]. The CSRL has two *CH,* online platforms, and a simulation lab in Santiago de Chile. The *CR* has the strength of being personalized to the customer segment, and personalization is essential for customer satisfaction [33]. The power of the *RS* is that the principal investigator has been granted government funding to execute computational chemistry research. The CSRL has *KR,* such as simulation computers, researchers, students, and funds. Research and development is one of the *KA* that enables growing knowledge and problem resolution. The CSRL has one *KP,* a private university that allowed the installation of the simulation lab. This partnership is essential to apply for government funding. The *CSE* of the CSRL had an equilibrium between fixed and variable costs. Both costs are covered by granted funds.

One weakness identified for *CS* is knowledge focalization, meaning the needs are covered just for a small group. This focalization is also present in the *VP,* which focuses only on academics. Regarding *CH*, the lab has no social media profiles where one can communicate activities and create content. The *CR* is personalized, which requires time and resources that may increase costs. The only monetary income in *RS* comes from government funds. This restricts the scope of action, which may negatively affect the opportunities. Also, the *KR is* weakened by more than one monetary income. *KA,* like networking and marketing, are not in execution; these may decrease the chance of getting to other researchers, labs, and students. The absence of social media facilitates the nonexistence of a marketing strategy. Only one *KP* is identified. This makes the lab vulnerable to any change that may impact the execution of the project. The funds obtained are a fixed budget, not allowing unexpected changes in the *CSE.*

Opportunities and threats correspond to external analysis, shown in Figure 2. SWOT analysis integrates internal (strengths/weakness) and external analysis, which is essential for strategy planning [34], [35]. One way to plan a strategy is by analyzing the strengths and weaknesses of the organization to identify the corporate identity [20]. Also, it is essential to identify threats and opportunities involving employees' knowledge to improve participative planning [21]. A TOWS matrix analysis matches threats and opportunities with strengths and weaknesses to trace a planned strategy for maximizing strengths-opportunities and minimizing weaknesses-threats [36].

S	W
1. Simulation knowledge 2. Published papers 3. Online and presential 4. Personalized 5. Funds granted/Lab faculty 6. Simulation lab 7. Project execution 8. University sponsorship 9. Overhead costs covered	1. Knowledge focalized 2. Only academics 3. No lab RRSS 4. Focalized 5. Only one source 6. One source of funds 7. No marketing strategy 8. Vulnerability to partner decisions 9. No funds for uncertainty
O	**T**
1. Applied science researchers 2. Book, Intellectual property 3. Collaborator lab 4. Relocation 5. Services/donations 6. New computer 7. Invitation to TV shows 8. International partnership 9. Costs covered by investors	1. Retirement 2. Data privatization 3. No connection & transport 4. Location 5. No funds transfer 6. Natural disaster 7. Lab closing 8. Bankrupt/Selling 9. Increase costs dramatically

Figure 2. SWOT analysis for each block of the business model. 1 Customer segment (CS). 2 Value proposition (VP). 3 Channels (CH). 4 Customer relationships (CR). 5 Revenue streams (RV). 6 Key resources (KR). 7 Key activities (KA). 8 Key partners (KP). 9 Cost structure (CSE)

The BMC for the CSRL outlined a comprehensive framework for its functioning. The model focused on academic researchers as its primary customer segment, offering a value proposition of enhancing research productivity. The lab utilizes online platforms and a physical facility for communication while establishing personalized customer relationships. Revenue streams come from collaborations, key partners (including private universities), and government funding. Key resources encompass simulation computers, researchers, and funds, enabling crucial activities like research and development, marketing, and networking. The strengths, weaknesses, opportunities, and threats (SWOT) analysis revealed strengths in simulation knowledge, successful publications, personalized customer relationships, and secured government funding. However, areas for improvement lie in limited knowledge and value proposition focus, absence of social media presence, reliance on government funding, and underutilized key activities. The lab's sustainability is tied to its partnership with a private university, yet it remains vulnerable to changes and needs a diversified income source. Balancing fixed and variable costs is essential in managing the cost structure. Overall, the CSRL's well-designed business model presents opportunities for growth and collaboration while necessitating strategic adjustments to address its weaknesses and ensure long-term success.

After designing the business model (Figure 1) and conducting the internal/external analysis (Figure 2), the number of published research articles from 1990 and 2022 were analyzed in four significant areas on Scopus databases.

During this period, around half of the research articles on computational simulation were concentrated in mathematics, physics, chemistry, and biology, as illustrated in Figure 3. Various factors may account for the substantial volume of research articles in the mathematical domain. Factors such as the broad applicability of mathematical models, a more expedited publication process, and fewer resource demands for theoretical experimentation might contribute to the higher count of research articles compared to experimental fields. Conversely, the biology field needed more published research articles that utilized computational simulation techniques.
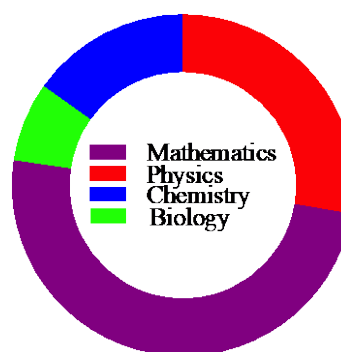

Figure 3. Computational simulation research articles published between 1990 and 2022 in Scopus databases

The average annual growth rate of publications was calculated to discern which central area grew the most and establish a trend. Figure 4 shows the publication's average annual growth rate for four periods. From 1990 to 1999, chemistry had the most significant publication growth rate (8%) in comparison to biology (5%), physics (4%), and mathematics (3%). From 2000 to 2009, biology had the greatest publication growth rate (13%) in comparison to mathematics (12%), physics (8%), and chemistry (8%). From 2010 to 2019, chemistry had the most significant publication growth rate (11%) in comparison to physics (10%), mathematics (9%), and biology (7%). From 2020 to 2022, chemistry had the greatest publication growth rate (16%) in comparison to physics (8%), mathematics (8%), and biology (10%). From the four periods analyzed, computational simulation in chemistry had three periods trending the growth of published articles research, 1990-1999, 2010-2019, and 2020-2022. External factors and internal factors have an impact on the growing rate. The increase in chemistry publications can be attributed to the ongoing requirement for developing new products using sustainable methods. Computational chemistry plays a pivotal role by efficiently simulating chemical reactions [37] and predicting properties before synthesis, resulting in significant time and computational resource savings [38].

The upward trajectory of chemistry publications mirrors the field's commitment to innovation and sustainability, with computational chemistry as a transformative tool that accelerates progress while optimizing resource utilization.
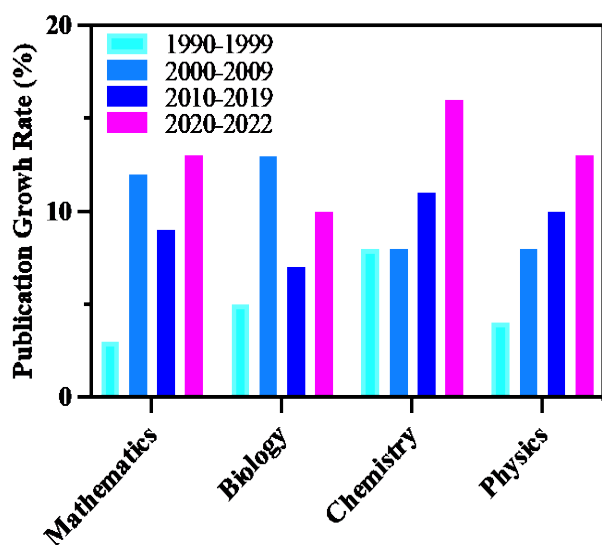

Figure 4. Growth publication trends in the four major areas

Following the analysis of the four primary areas, the articles published in various computational chemistry applications were examined, as shown in Figure 5. Specifically, the analysis investigated simulation, algorithm development, database utilization, and data analysis, scrutinizing the number of research articles published on Scopus databases from 1990 to 2022. Notably, simulation, algorithm development, database utilization, and data analysis demonstrated comparable levels of research article output during this period. In contrast, material design, molecular modeling, chemical reaction analysis, and drug discovery domains exhibited relatively fewer research articles published within the same timeframe.

Remarkably, a common trend emerged across all these applications, with a notable upswing in published research articles around the 2000s. This period was marked by substantial breakthroughs in computational simulations, fueled by advancements such as the introduction of graphics processing units (GPUs) in 1999, the emergence of quantum simulations [39], the deployment of the IBM ASCI white supercomputer in 2000, and the development of algorithms designed to mitigate computational expenses [40]. These advancements collectively contributed to the growth and proliferation of research articles across the computational chemistry landscape.
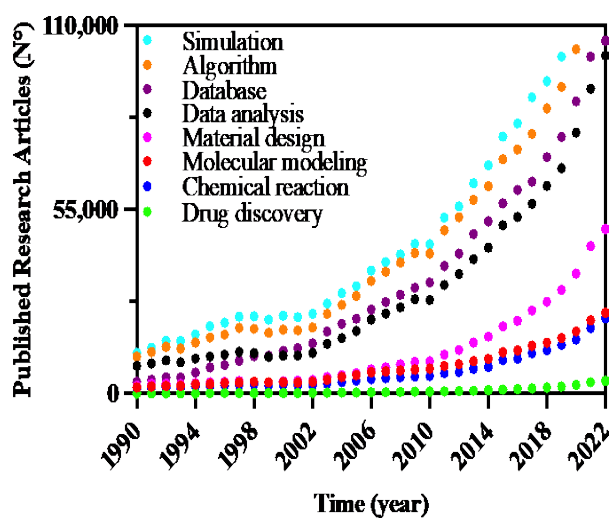

Figure 5. Computational chemistry research articles published in different applications

The investigation focused on determining the areas with the most pronounced expansion and establishing an overarching trajectory across various applications. Figure 6 provides a comprehensive visualization of publications' mean annual growth rates across four distinct timeframes. Notably, during the period spanning from 1990 to 1999, both drug discovery and database fields exhibited remarkable growth rates of 13% each. Subsequently, spanning from 2000 to 2009, the drug discovery domain showcased the most substantial surge, with a growth rate of 17%. Similarly, from 2010 to 2019, drug discovery sustained its upward trajectory, with the highest growth rate observed at 15%. Remarkably, between 2020 and 2022, drug discovery experienced an accelerated expansion, reaching an unprecedented growth rate of 21%. Collectively, drug discovery consistently demonstrated the most robust growth across all examined periods. The increase in this growth pattern can be attributed to a range of complex factors. Particularly noteworthy is the heightened alarm over the antimicrobial resistance crisis [41], which has emerged as a central determining factor with significant implications. Beyond this, other elements might also contribute to this trend, such as technological advancements, changing consumer preferences, and evolving regulatory frameworks. As these influences intertwine, they create a dynamic landscape that shapes the observed growth pattern. Considering these multifaceted dynamics, addressing the antimicrobial resistance crisis could be a step toward sustainable growth while necessitating an approach encompassing various sectors and stakeholders.
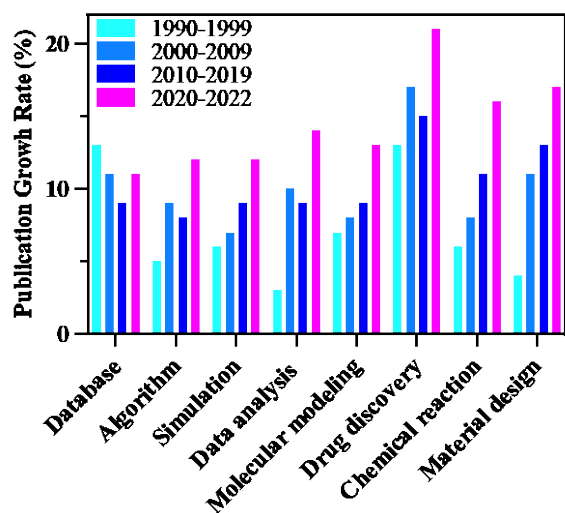
Figure 6. Growth publication trends in computational chemistry applications

4. Conclusion

This study was set out to develop a business model for a computational simulation research lab and a strategic SWOT analysis. The study also aimed to identify trends in published research articles related to computational simulation. The present study presents a meticulously crafted business model tailored to a research laboratory, delineating pivotal activities, requisite resources, and strategic partnerships. Through a comprehensive SWOT analysis, this investigation has unearthed a singular determinant within each facet of the business model, thereby providing a roadmap for prudent resource allocation and time optimization. Essential findings, chemical simulation, outperforms more published research articles than other disciplines. Specifically, the vanguard appears to be in drug discovery—a prevailing trend with promising potential within chemical applications. The innovative approach encompassing business model design, rigorous SWOT analysis, and astute market research on publication trends demonstrates its efficacy as an invaluable suite of strategic instruments poised for seamless integration into research activities. Although this study was limited to conceptualization, variable identification, and scrutiny of secondary data, it inevitably precluded a firsthand evaluation of business model implementation. Undeterred by these inherent limitations, this inquiry proffers a resounding proposition: business model designing, meticulous market analysis, and strategic planning are pivotal pillars underpinning the triumphant execution of research projects.

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