Global Journal of Chemistry
Vol. 1 No.1 2026 Page 11-19
E-ISSN: XXXX-XXXX, DOI: 10.XXXXX/XXXX

A Conceptual Model for the Development of Chemical Materials Based on Green Chemistry and Cheminformatics

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Article Info

Received : X Month Year
Revised : X Month Year
Accepted : X Month Year

Keyword:

Green chemistry;
Cheminformatics;
Chemical material Development;
Conceptual model;
Sustainable chemistry.

ABSTRACT

This study aims to develop a conceptual model for chemical material development based on green chemistry and cheminformatics. The issue addressed in this study concerns the gap between sustainability principles and laboratory practices, where material development often still relies on trial-and-error methods, limited toxicity assessment, and insufficient use of molecular data at the early design stage. This study used an exploratory qualitative approach with a constructivist grounded theory design. Data were collected from 12 to 18 purposively selected participants, including chemistry lecturers, material researchers, laboratory practitioners, curriculum developers, and academics with experience in green chemistry, computational chemistry, material design, or cheminformatics. Data collection involved semi-structured interviews, non-participant observation, documentation, and triangulation. The findings reveal four main themes: sustainability orientation in chemical material design, limitations of conventional laboratory practice, the role of molecular data in material candidate selection, and the need for an integrated conceptual model. The study proposes a model consisting of five components: material need identification, mapping of green chemistry principles, cheminformatics-based analysis, candidate selection, and reflective evaluation. These findings contribute to the development of an integrative framework that connects green chemistry, chemical data intelligence, and sustainable material design. The study implies that chemistry education, laboratory policy, and research practice should strengthen the use of molecular data and sustainability indicators before experimental work begins.

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1. Introduction

The development of modern chemistry shows a clear shift from conventional synthesis toward safer, more efficient, and more sustainable chemical materials. This shift occurs because chemical production and use do not only generate technical benefits. They also create risks for human health, laboratory safety, and environmental quality. Green chemistry offers a relevant framework because it emphasizes waste prevention, efficient material use, toxicity reduction, safer solvent selection, and environmentally responsible design from the earliest stage of chemical

development. Mammino (2023) explains that green chemistry has a close relationship with computational chemistry because molecular design, property prediction, and hazard evaluation can be conducted before laboratory experiments begin. This view strengthens the position of green chemistry as a conceptual basis for developing chemical materials that are not only functional but also ecologically responsible.

At the global level, the demand for safer and more sustainable materials continues to increase as industries, universities, and research institutions face stronger pressure to reduce environmental impacts. Chemical material development can no longer depend only on trial-and-error approaches that require large amounts of solvents, reagents, energy, and time. Weber et al. (2021) argue that chemical data intelligence can support sustainable chemistry because chemical data can help researchers select reaction pathways, evaluate alternative substances, and estimate potential risks at an early stage. Derbenev et al. (2022) also show that green and sustainable chemistry software can assist researchers in evaluating sustainability metrics, selecting safer solvents, and designing safer experiments. These findings indicate that sustainability in chemistry requires an integration of normative principles, molecular data, and computational technology.

In the national context, the development of sustainability-based chemical materials still faces challenges in education, research, and laboratory practice. Many chemistry learning activities and material research projects still focus on synthesis success, procedural accuracy, and final experimental results. Issues such as material toxicity, environmental safety, atom economy, waste footprint, and predictive data are not always placed at the center of research planning. Marcelino et al. (2023) show that green chemistry teaching requires clear didactic strategies so that sustainability is not understood only as a theoretical concept, but also applied in scientific practice. Da Silva Júnior et al. (2024) add that green and sustainable chemistry education needs to be designed inclusively so that students can connect chemical concepts with social and environmental responsibility.

Field-level problems also appear in the selection process of chemical material candidates, which often depends on researcher intuition, laboratory experience, and repeated testing. This practice can increase the use of hazardous substances, expand laboratory waste, and extend the material development process. Cheminformatics offers an important opportunity to respond to this issue through molecular structures, chemical descriptors, toxicity prediction, physicochemical property data, and structure-activity relationships. Djoumbou-Feunang et al. (2023) explain that cheminformatics and artificial intelligence can accelerate molecular discovery through virtual screening, candidate optimization, and the reduction of inefficient early-stage experiments. Bărbulescu and Barbeș (2025) also show that cheminformatics can support the analysis of polymer additives, compound clustering, and environmental impact assessment in polymeric materials.

Although green chemistry and cheminformatics have strong potential to complement each other, previous studies tend to discuss both fields separately. Green chemistry is often examined as an ethical, pedagogical, and practical principle for reducing environmental impact. Cheminformatics is more often positioned as a computational tool for property prediction, molecular discovery, or chemical structure classification. Saxe et al. (2022) demonstrate the importance of incorporating green chemistry principles at the early stage of product design so that sustainability considerations appear from the conceptual phase. Amoneit et al. (2024) emphasize that green chemistry needs to move beyond the twelve principles by incorporating responsible research and innovation. However, few studies have developed an integrated conceptual model that explains how green chemistry principles can be translated into material design indicators through cheminformatics data.

Based on this gap, this study aims to develop a conceptual model for chemical material development based on green chemistry and cheminformatics. The study focuses on the relationship between sustainability principles, molecular characteristics, material property

prediction, safety indicators, experimental efficiency, and material candidate selection. Theoretically, this study contributes to strengthening an integrative framework between green chemistry, chemical data intelligence, and data-driven material design. Practically, the model can help lecturers, researchers, students, and laboratory practitioners develop a more systematic early-stage workflow before conducting experiments. Mammino (2025) emphasizes that green chemistry needs to be bridged with environmental chemistry so that future chemists understand the relationship between pollutant sources, material impacts, and prevention strategies. Nwafor et al. (2025) also show that electronic lab notebooks can support more sustainable laboratory practices through experiment documentation and systematic data integration.

2. Materials and Methods

The author(s) must describe exactly the steps: what and how experiments were run, what, how This study used an exploratory qualitative approach with a constructivist grounded theory design. This approach was selected because the study aimed to develop a conceptual model, not to test statistical relationships among variables. The research focused on understanding experiences, scientific considerations, interpretive processes, and the ways academics, researchers, and laboratory practitioners make sense of chemical material development based on green chemistry and cheminformatics. Lim (2025) explains that qualitative research is suitable for understanding complex phenomena because it explores meaning, process, context, and participant experience in depth. Through this approach, the study can explain how sustainability principles are translated into material selection, molecular data use, and material development workflows.

The study was conducted from 15 November 2025 to January 2026 at selected universities and chemistry research laboratories in Indonesia that had learning, research, or material development activities related to green chemistry, computational chemistry, and material analysis. The research sites were selected purposively because they had direct relevance to the focus of the study. Part of the data collection was conducted offline in laboratories, chemistry study programs, and material research units. Some interviews were conducted online to reach informants with specific expertise in cheminformatics, molecular design, material property modeling, or sustainability evaluation. This strategy was used to obtain varied data from institutions with different levels of readiness and experience in implementing sustainable chemistry principles.

The participants consisted of chemistry lecturers, material researchers, laboratory practitioners, chemistry curriculum developers, and academics with experience in green chemistry, computational chemistry, material design, or cheminformatics software. Informants were selected using purposive sampling based on several criteria. First, they had at least two years of experience in chemistry education, research, or laboratory practice. Second, they understood material safety, laboratory sustainability, or material development issues. Third, they had been involved in the design, synthesis, analysis, evaluation, or modeling of chemical materials. Ahmad and Wilkins (2025) state that purposive sampling needs to be designed coherently from research objectives, informant selection, data collection, and reporting. Snowball sampling was used in a limited way to identify additional informants with specific expertise in toxicity prediction, molecular modeling, or chemical data integration.

The planned number of informants ranged from 12 to 18 people and could be stopped when the data reached saturation. Saturation refers to the condition in which additional interviews no longer produce new substantive categories, themes, or information relevant to the research focus. Hennink and Kaiser (2022) show that many qualitative studies with relatively homogeneous populations can reach saturation within 9 to 17 interviews. The number of informants in this study remained flexible because data quality was prioritized over participant quantity. Therefore, the researcher considered the depth of information, the diversity of informant backgrounds, and the

adequacy of data to construct a conceptual model that explains chemical material development based on green chemistry and cheminformatics.

Data were collected through semi-structured interviews, non-participant observation, documentation, and data triangulation. Semi-structured interviews were used to explore informants' experiences in selecting materials, assessing environmental risks, using chemical data, considering toxicity, and determining the feasibility of material candidates before synthesis. The interview guide was developed based on several initial themes: green chemistry principles, molecular data use, material selection practices, material property prediction, and the need for a conceptual model. Non-participant observation was conducted in learning or laboratory activities related to material selection, solvent use, experiment recording, chemistry software use, and material risk assessment. Documentation was conducted by reviewing syllabi, practicum modules, laboratory SOPs, material safety guidelines, research articles, experiment notes, and workflow documents for material development. Dalglish et al. (2020) explain that document analysis can strengthen qualitative research because it helps researchers understand the content, process, and context of practices that may not fully appear in interviews.

Data validation was conducted through source triangulation, method triangulation, member checking, and audit trail. Source triangulation was carried out by comparing information from lecturers, researchers, laboratory practitioners, curriculum developers, and institutional documents. Method triangulation was conducted by comparing interview results, observation notes, and documents. Member checking was conducted by sending summaries of interview results or early interpretations to informants to confirm the fit between their experiences and the researcher's interpretation. An audit trail was maintained by keeping records of research decisions, category changes, analytical memos, interview guides, document lists, and theme development processes. Ahmed (2024) explains that credibility, transferability, dependability, and confirmability in qualitative research can be strengthened through triangulation, member checking, researcher reflexivity, systematic documentation, and audit trail.

Data analysis was conducted through open coding, axial coding, and selective coding, combined with reflexive thematic analysis. In the open coding stage, the researcher identified meaning units from interview transcripts, observation notes, and research documents. In the axial coding stage, conceptually related codes were grouped into categories, such as sustainability principles, material candidate selection, molecular property prediction, toxicological risk, experimental efficiency, laboratory readiness, and cheminformatics data use. In the selective coding stage, the main categories were integrated to construct propositions and a conceptual model. Braun and Clarke (2021) emphasize that high-quality thematic analysis must maintain coherence between research questions, theoretical position, coding process, and theme development. Nicmanis (2024) also emphasizes the importance of reflexivity in qualitative analysis because researchers need to recognize the influence of prior knowledge, assumptions, and analytical decisions on data interpretation.

3. Results and Discussions

The findings show that participants understand the development of chemical materials based on green chemistry and cheminformatics as an increasingly important need in chemistry education, research, and laboratory practice. Data from interviews, observations, and document analysis produced four main themes: sustainability orientation in chemical material design, limitations of conventional laboratory practice, the role of molecular data in material candidate selection, and the need for a conceptual model that integrates green chemistry and cheminformatics. These four themes are connected. They show that chemical material development cannot rely only on technical performance. It must also consider safety, efficiency, environmental impact, and data traceability from the earliest stage of design.

The first theme shows that green chemistry is understood as both an ethical and a practical framework for chemical materials development. Most participants stated that green chemistry principles have not fully become the main basis for experimental planning, although they recognized the importance of waste reduction, safer solvent selection, and material efficiency. One chemistry lecturer stated, "We often teach green chemistry concepts, but in laboratory practice, the implementation is still gradual because of limited materials, equipment, and working habits." This statement shows a gap between conceptual understanding and practical implementation in the laboratory. Observation results also showed that several practical activities still used older procedures that did not fully consider waste minimization and material risk evaluation.

The second theme relates to the limitations of conventional laboratory practice. Participants explained that material development often relied on repeated testing based on the researcher's experience, previous references, and available chemicals in the laboratory. This pattern helped in basic learning contexts, but it was less efficient for material research that required accuracy, safety, and sustainability. A material researcher stated, “Sometimes we choose materials because they have been commonly used in previous studies, not because they have truly been compared in terms of toxicity or environmental impact.” This finding indicates that material selection is still often shaped by academic habits and resource availability, rather than by a structured assessment system.

The third theme shows that cheminformatics is viewed as a promising approach to strengthen decision-making in chemical material development. Participants with experience in computational chemistry argued that molecular data, chemical descriptors, physicochemical property prediction, and toxicity models can help screen material candidates before synthesis. One participant explained, “If molecular data can be read earlier, we can reduce unnecessary trials. This is important for material efficiency and work safety.” This statement indicates that cheminformatics is not only a prediction tool. It also functions as an early mechanism to reduce risk, cost, and experimental waste. Research documentation also showed that some laboratories had used chemistry software, but its use was still mostly limited to structure visualization or basic property calculation.

The fourth theme shows the need for a conceptual model that connects green chemistry principles with cheminformatics-based analysis. Participants stated that there was no simple workflow that could be used consistently to assess material candidates based on sustainability principles and molecular data. A curriculum developer stated, “Students need a clear model. They should know when to consider toxicity, when to examine molecular structure, and how to connect all of that with green chemistry principles.” This finding suggests that a conceptual model is needed not only for research, but also for chemistry education, curriculum development, and the formation of a more responsible laboratory culture.

Based on the overall findings, the conceptual model emerging from the data consists of five main components. The first component is the identification of material needs and expected chemical functions. The second component is the mapping of relevant green chemistry principles, such as waste prevention, atom economy, safer solvent use, and the design of less toxic materials. The third component is cheminformatics analysis through molecular structure, chemical descriptors, property prediction, and toxicity potential. The fourth component is material candidate selection based on safety, efficiency, availability, and environmental impact. The fifth component is reflective evaluation through documentation, laboratory validation, and workflow improvement. This model indicates that sustainable chemical material development should begin at the conceptual stage, not only after laboratory experiments have been completed.

Discussion

The findings strengthen the view that green chemistry should be positioned as a core framework for modern chemical materials development. Participants not only understood green

chemistry as an environmental principle. They also viewed it as a scientific way of thinking that affects material selection, experimental design, waste management, and laboratory safety. This finding is consistent with Mammino (2023), who explains that green chemistry is closely connected to computational chemistry because material evaluation can begin at the molecular design stage. It also supports Kurul et al. (2025), who emphasize that green chemistry principles are important for building a more sustainable future for chemistry.

However, the findings also show that the implementation of green chemistry in laboratories has not yet become fully systematic. Participants were aware of the importance of sustainability, but experimental practice was still influenced by old procedures, material availability, and academic habits. This finding reveals a gap between conceptual knowledge and operational practice. Marcelino et al. (2023) explain that green chemistry teaching requires clear didactic strategies so that students and practitioners do not only understand the principles, but can also apply them in scientific activities. Da Silva Júnior et al. (2024) also emphasize that sustainable chemistry education should connect chemical concepts to social and environmental responsibility.

The finding on the limitations of conventional laboratory practice shows that trial-and-error remains a common pattern in material development. This pattern can be understood as part of the experimental tradition in chemistry. However, it becomes less adequate when research demands efficiency, safety, and lower environmental impact. Weber et al. (2021) explain that chemical data intelligence can help overcome these limitations by using chemical data to select reaction pathways, evaluate alternative materials, and estimate risk. Therefore, the findings support the idea that chemical data should be incorporated into the material design process earlier, not only after experiments have produced final data.

The role of cheminformatics identified in this study shows an opportunity to strengthen material candidate selection. Participants viewed molecular structures, chemical descriptors, toxicity prediction, and physicochemical properties as useful tools to reduce unnecessary experiments. This finding is in line with Djoumbou-Feunang et al. (2023), who show that cheminformatics and artificial intelligence can accelerate molecular discovery through virtual screening and candidate optimization. Bărbulescu and Barbeș (2025) also show that cheminformatics can be used to analyze polymer additives and assess potential environmental impacts. The difference in this study lies in its focus on cheminformatics not only as a technical tool, but also as part of a conceptual model for more sustainable chemical material development.

The findings also indicate that the integration of green chemistry and cheminformatics has not fully become an established framework in education and laboratory practice. Green chemistry often appears as a normative principle, while cheminformatics appears as a computational tool. These two areas are not always connected in a practical workflow. Saxe et al. (2022) show the importance of incorporating green chemistry principles at the early stage of product design. Amoneit et al. (2024) add that green chemistry needs to move toward responsible research and innovation so that technical, social, ethical, and environmental dimensions can be considered together. This study offers a new perspective by positioning the integration of green chemistry and cheminformatics as a conceptual model that can support both research and learning.

Theoretically, the findings expand the understanding of the relationship between sustainable chemistry and data-driven material design. The proposed model shows that sustainable chemical material development requires not only green chemistry principles, but also molecular data that can support more rational material selection. This means that sustainability should not be treated only as a final evaluation of material impact. It should become part of the design process from the beginning. In this sense, the study strengthens the position of chemical data intelligence as a bridge between green chemistry theory and material development practice.

Practically, the findings have implications for lecturers, researchers, students, and laboratory managers. The proposed conceptual model can be used as an initial guide for designing chemical material development workflows. Lecturers can use it to strengthen learning in green and

computational chemistry. Researchers can use it to screen material candidates before conducting experiments. Laboratory managers can use it to improve safety culture, material efficiency, and experiment documentation. Nwafor et al. (2025) show that electronic lab notebooks can support more sustainable laboratory practices by enabling the recording of experiments and integrating data. This finding is relevant to the needs of modern laboratories that require more structured documentation and evaluation systems.

A critical reflection from this study shows that implementing a green-chemistry and cheminformatics-based model still requires human-resource readiness, software access, data infrastructure, and changes in laboratory culture. Not all laboratories have access to computational tools, molecular databases, or cheminformatics training. Some practitioners also still view green chemistry as an additional requirement rather than an essential part of experimental design. Therefore, future studies should test this conceptual model in different laboratory contexts, such as teaching laboratories, material research laboratories, pharmaceutical laboratories, polymer research, and agrochemical development. Further research can also develop evaluation instruments, learning modules, or technical guidelines to measure how far green chemistry and cheminformatics principles are actually implemented in chemical material development.

4. Conclusions

This study concludes that the development of chemical materials based on green chemistry and cheminformatics requires an integrated conceptual framework that connects sustainability principles, molecular data, safety indicators, experimental efficiency, and material candidate selection. The findings show that green chemistry is not only understood as an environmental principle, but also as a scientific framework that guides safer material design, waste reduction, solvent selection, and laboratory responsibility. However, the implementation of these principles remains uneven because laboratory practices are still shaped by old procedures, material availability, and trial-and-error approaches. Cheminformatics offers a strategic role in addressing this gap by supporting early-stage screening through molecular structures, chemical descriptors, property prediction, and toxicity assessment.

Theoretically, this study contributes to the literature by positioning chemical data intelligence as a bridge between green chemistry principles and data-driven material design. Practically, the proposed conceptual model can guide lecturers, researchers, students, and laboratory managers in developing a more systematic workflow before synthesis and laboratory testing. From a policy perspective, the findings suggest the need to strengthen green chemistry and cheminformatics integration in chemistry curricula, laboratory standards, research protocols, and institutional sustainability policies. Future studies should test this conceptual model in different laboratory contexts, develop measurable indicators for its implementation, and design learning modules or technical guidelines that can support sustainable chemical material development.

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