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Integration of Green Chemistry and a Data-Driven Approach in the Development of Sustainable Nanomaterials

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ABSTRACT

This study aims to explore the integration of green chemistry and a data-driven approach in the development of sustainable nanomaterials. The issue is important because nanomaterial synthesis increasingly requires safer, more efficient, and environmentally responsible processes, while many laboratories still face challenges in reproducibility, data management, and sustainability assessment. This study used a qualitative case study design involving researchers, laboratory analysts, postgraduate students, and practitioners engaged in nanomaterial synthesis, green synthesis, material characterization, or experimental data processing in Indonesian research laboratories. Data were collected through semi-structured interviews, limited observation, and documentation, then analyzed using thematic analysis. The findings reveal six main themes: green chemistry as laboratory responsibility, reproducibility challenges in green synthesis, the role of data in reducing trial-and-error practices, emerging interest in machine learning, the need for early safety and sustainability assessment, and the importance of research culture in supporting sustainable nanomaterial development. The study shows that the integration of green chemistry and data-driven approaches is not merely a technical matter, but a socio-scientific process shaped by laboratory habits, institutional support, data literacy, and interdisciplinary collaboration. These findings contribute to sustainable nanomaterial studies by offering a qualitative understanding of how researchers interpret, negotiate, and apply sustainability principles in real laboratory contexts. The study implies that laboratories and institutions need stronger data documentation systems, green chemistry training, and safe and sustainable by design guidelines to support responsible nanomaterial innovation.

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1. Introduction

The development of sustainable nanomaterials has become an important issue in modern chemical research because the demand for functional materials continues to increase in energy, health, environmental, food, and industrial sectors. Nanomaterials offer advantages in particle size, surface area, reactivity, and application flexibility. However, their synthesis can create environmental problems when it still depends on toxic solvents, high energy consumption, hazardous chemicals, and reaction waste that is difficult to control. Gupta et al. (2023) explain that green nanomaterial synthesis has developed as a response to the limitations of conventional methods that are energy-intensive and environmentally risky. Ying et al. (2022) also emphasize that the use of plants, microorganisms, and biomolecules as reducing or stabilizing agents can support safer nanomaterial development. However, this practice still faces challenges related to reproducibility, particle stability, morphology control, and product quality consistency.

In the Indonesian context, this issue is relevant because nanomaterial research increasingly uses local biological resources, plant extracts, biomass waste, and natural materials as the basis for green synthesis. This potential aligns with the principles of green chemistry, which emphasize waste prevention, atom economy, safer substances, low-toxicity product design, and energy efficiency. Mulyana et al. (2024) show that lime can be used as a bioreductant in silver nanoparticle synthesis, which indicates that local natural materials can support more environmentally friendly material development. Dikshit et al. (2021) also state that plant- and microorganism-based nanoparticle synthesis has practical value in various sectors, but it still requires stricter process control. This condition shows that the challenge of sustainable nanomaterial development lies not only in successful synthesis, but also in the ability of laboratories to manage material variation, experimental data, safety, and process sustainability.

A common problem in the field is the strong dependence on trial-and-error methods in determining synthesis parameters, such as pH, temperature, reaction time, precursor concentration, solvent type, and bioreductant composition. This process can consume large amounts of materials, energy, and time when it is not supported by a reliable data system. Jia et al. (2021) explain that machine learning can accelerate nanomaterial design and discovery by analyzing patterns from experimental data. Kumar et al. (2021) also show that data-based approaches can be used to select more sustainable solvents in porous material synthesis. In a recent study, Ye et al. (2025) demonstrate that machine learning can optimize the green synthesis of iron sulfide nanoparticles from biomass while improving heavy metal adsorption performance. These findings show that a data-driven approach can strengthen green chemistry principles because it can reduce repeated experiments, accelerate optimization, and help researchers make evidence-based decisions.

The integration of green chemistry and a data-driven approach also has social, educational, and research culture dimensions. In laboratory practice, researchers deal not only with technical procedures, but also with how they understand risk, read data, select parameters, and interpret sustainability as a scientific value. Ji et al. (2021) emphasize the importance of nanomaterial databases in supporting design, material selection, and risk assessment. Furxhi et al. (2022) extend this idea through a sustainable and safe-by-design approach that places safety and sustainability at the early stage of nanomaterial development. Furxhi et al. (2023) further show that data that are findable, accessible, interoperable, and reusable can support the development of intrinsic hazard criteria for nanoforms. Therefore, sustainable nanomaterial development needs to be understood as a scientific process that combines green chemistry principles, data literacy, safety ethics, and ecological responsibility.

Previous studies have widely discussed green synthesis, nanomaterial applications, machine learning, databases, and risk assessment. Zhang et al. (2023) review the importance of sustainable nanomaterials for biomedical applications. Tripathy et al. (2024) explain that the convergence of nanotechnology and machine learning can support synthesis, characterization, and property optimization. Xiao et al. (2025) argue that machine learning can assist the analysis of biological safety and sustainability of metal nanomaterials. Saha (2025) also shows that nanoinformatics can strengthen safer nanomaterial design through the use of large-scale data. However, most of these studies focus on technical, computational, or conceptual review aspects. Few qualitative studies have explored how researchers interpret the integration of green chemistry and data-driven approaches, how decision-making processes occur in laboratories, and how sustainability values are negotiated under limitations in facilities, data, evaluation standards, and research culture.

Based on this gap, this study aims to deeply understand the integration of green chemistry and data-driven approaches in the development of sustainable nanomaterials. The study focuses on the experiences, meanings, strategies, and challenges faced by researchers or laboratory practitioners when applying green chemistry principles, using experimental data, and assessing material safety and sustainability from the design stage. Parab et al. (2025) emphasize that the future of nanotechnology needs to move toward greener, more economical, and lower-toxicity practices. Chatzipanagiotou et al. (2025) also show that the implementation of safe and sustainable by design still faces challenges due to differences in assessment tools, data requirements, and functional unit definitions. Therefore, this study is expected to provide a theoretical contribution to the development of sustainable nanomaterial studies from a qualitative perspective, as well as practical contributions for laboratories, educational institutions, and policymakers in designing research systems that are safer, more efficient, data-based, and aligned with green chemistry principles.

2. Materials and Methods

This study uses a qualitative approach with a case study design. This approach was selected because the study does not aim to test statistical relationships among variables, but to understand in depth the processes, experiences, considerations, and challenges faced by researchers in integrating green chemistry principles and data-driven approaches in the development of sustainable nanomaterials. A case study design is appropriate because the issue is situated in a real laboratory context and involves scientific decision-making processes, the use of experimental data, facility limitations, and considerations of safety and sustainability. Priya (2021) explains that case studies allow researchers to understand complex phenomena based on their social, institutional, and practical contexts. Thus, this approach is relevant for revealing how the integration of green chemistry and data-driven approaches is understood, applied, and negotiated by nanomaterial researchers.

This study will be conducted in chemistry laboratories, nanomaterial laboratories, or material research centers at universities and research institutions in Indonesia that conduct research on nanomaterial synthesis, green synthesis, material characterization, or experimental data use. The study is planned to be conducted over four months, from May to August 2026, covering instrument preparation, data collection, data verification, analysis, and findings development. The research subjects include principal investigators, lecturers or academics in material chemistry, laboratory analysts, postgraduate students involved in nanomaterial synthesis, and researchers or practitioners who use computational approaches, machine learning, or experimental data processing. The estimated number of informants ranges from 12 to 18 people, but this number may be adjusted based on data depth and information saturation. Informants will be selected using purposive sampling because the study requires participants with direct experience and relevant knowledge of the research topic. Campbell et al. (2020) state that purposive sampling is appropriate in qualitative research because it enables researchers to select participants who can provide rich information according to the study focus.

The informant criteria include four main requirements. First, informants must have experience in researching, synthesizing, characterizing, or developing nanomaterials. Second, informants must understand or have applied green chemistry principles, such as the use of safer solvents, natural materials, bioreductants, energy efficiency, or laboratory waste reduction. Third, informants must have used experimental data, analytical software, machine learning, material databases, or computational approaches in research decision-making. Fourth, informants must be willing to participate in interviews and provide information based on real experience. In addition to purposive sampling, snowball sampling may be used when initial informants recommend other researchers with more specific experience, such as researchers who develop nanomaterial property prediction models or those who handle laboratory safety and sustainability issues. Bouncken et al. (2025) explain that participant selection in qualitative studies needs to consider the suitability of the level of analysis, information variation, and data saturation so that the findings have conceptual depth and relevance.

Data will be collected through semi-structured interviews, limited observation, documentation, and data triangulation. Semi-structured interviews will serve as the main data collection technique because they allow informants to explain their experiences, views, strategies, and constraints openly while remaining aligned with the research focus. Interview questions will cover informants' understanding of green chemistry, experiences in nanomaterial synthesis, use of experimental data, selection of synthesis parameters, reproducibility challenges, safety considerations, and perceptions of data-driven approaches. Limited observation will be conducted to understand laboratory practices, synthesis workflows, experimental data recording, instrument use, and waste management. Documentation will involve the review of laboratory notes, synthesis protocols, safety documents, characterization reports, published articles, or experimental data permitted by the institution. The use of multiple data collection techniques is intended to provide a more complete understanding of the practices, meanings, and processes involved in integrating green chemistry with a data-driven approach.

Data validation will be conducted through source triangulation, method triangulation, member checking, and an audit trail. Source triangulation will compare information from principal investigators, laboratory analysts, postgraduate students, and data practitioners. Method triangulation will compare interview, observation, and documentation data. Member checking will be conducted by sending interview summaries or initial interpretations to informants to ensure that the meanings captured by the researcher match the informants' experiences. An audit trail will be maintained by storing research process notes, interview transcripts, observation notes, coding decisions, category changes, and analytical memos. Johnson et al. (2020) emphasize that the quality of qualitative research needs to be maintained through transparent design, documented analysis processes, and detailed explanations of research procedures. Ahmed (2024) also explains that trustworthiness in qualitative research can be strengthened through credibility, transferability, dependability, and confirmability.

Data will be analyzed using thematic analysis. This technique was selected because the study aims to identify patterns of meaning from informants' experiences regarding the integration of green chemistry and data-driven approaches in sustainable nanomaterial development. Kiger and Varpio (2020) explain that thematic analysis is suitable for identifying, analyzing, and reporting patterns of meaning in qualitative data. The analysis will be conducted in several stages. First, the researcher will repeatedly read interview transcripts and observation notes to understand the data context. Second, initial coding will be conducted on important statements, such as "selection of safer solvents," "instability of natural materials," "undocumented experimental data," "parameter optimization," "machine learning," "laboratory safety," and "process sustainability." Third, codes with related meanings will be grouped into categories. Fourth, categories will be developed into main themes, such as green synthesis practices, the role of data in decision-making, laboratory sustainability challenges, data infrastructure limitations, and the need for safe and sustainable by design. Fifth, themes will be reviewed by comparing raw data, analytical memos, and research objectives. Braun and Clarke (2021) emphasize that thematic analysis gives researchers flexibility to interpret patterns of meaning reflectively, as long as the analysis process is conducted systematically and transparently.

3. Results and Discussions

The findings show that the integration of green chemistry and a data-driven approach in sustainable nanomaterial development is understood by participants as a gradual and adaptive process rather than a fixed technical procedure. Most participants viewed green chemistry as an ethical and practical framework for reducing the environmental burden of nanomaterial synthesis. They associated green chemistry with the use of safer solvents, natural reducing agents, biomass-based materials, lower energy consumption, and better laboratory waste management. However, participants also stated that the implementation of green chemistry principles was often limited by the availability of instruments, the variability of natural materials, and the lack of standard operating procedures. One participant explained, “We want to use plant extracts or biomass because they are safer, but the composition is not always stable. The result can change from one batch to another” (P3). This statement indicates that sustainability in nanomaterial synthesis is not only related to material selection, but also to the capacity of laboratories to control uncertainty in the synthesis process.

The first major theme concerns the meaning of green chemistry as a form of laboratory responsibility. Participants did not define green chemistry only as a method for replacing hazardous chemicals. They understood it as a broader responsibility to design safer processes, reduce unnecessary experimentation, and minimize ecological risks. Several participants described that the decision to use natural materials was influenced by environmental concerns and the need to make research more relevant to local resources. One participant stated, “Using local biomass makes the research more meaningful because we do not only produce nanoparticles, but also try to reduce waste and use available resources” (P7). This finding suggests that green chemistry carries both scientific and socio-environmental meanings. In the Indonesian research context, the use of local biological resources also reflects an effort to connect laboratory innovation with national resource potential.

The second theme relates to the challenge of reproducibility in green nanomaterial synthesis. Participants reported that plant extracts, biomass waste, and natural reducing agents often produced different nanoparticle characteristics because their chemical composition depended on source, season, storage condition, and extraction method. This problem affected particle size, morphology, stability, and functional performance. Observation notes from laboratory activities also showed that some researchers still relied on repeated experimental adjustment to obtain desired material characteristics. One laboratory analyst noted, “The most difficult part is not only making the particles, but making them consistently. Sometimes the same formula gives a different result” (P2). This finding shows that reproducibility is a central issue in sustainable nanomaterial development. It also explains why green synthesis needs stronger data documentation and process control.

The third theme concerns the role of data in reducing trial-and-error practices. Participants stated that experimental data were valuable for identifying patterns among synthesis parameters, such as pH, temperature, precursor concentration, reaction time, solvent type, and bioreductant composition. However, not all laboratories had systematic data management. Some data were stored in personal notebooks, separate files, or unpublished reports. This made it difficult to reuse data for future experiments or computational modeling. One participant explained, “We have many experimental results, but they are scattered. If the data were organized, we could learn faster from previous experiments” (P5). Documentation analysis also showed that laboratory records often focused on successful results, while failed experiments were rarely archived in a structured format. This condition limits the development of data-driven research because machine learning and predictive modeling require complete, consistent, and reusable datasets.

The fourth theme highlights the emerging interest in machine learning and computational tools. Participants recognized that machine learning could help predict material properties, optimize synthesis parameters, and reduce unnecessary laboratory trials. Some participants had used basic statistical software, while others had begun exploring machine learning models for data interpretation. However, the adoption of data-driven methods remained uneven. Barriers included limited computational skills, lack of integrated databases, small sample sizes, and limited collaboration between chemists and data scientists. One postgraduate student stated, “We know machine learning can help, but our problem is the data. The data are not always enough, and not everyone knows how to process them” (P11). This finding indicates that the data-driven approach is not only a technological issue, but also a matter of research literacy, interdisciplinary collaboration, and institutional support.

The fifth theme concerns safety and sustainability assessment from the early stage of material design. Participants stated that nanomaterial research often focused on synthesis success and application performance, while safety, toxicity, life-cycle impact, and waste management received less attention. Some participants admitted that safety evaluation was usually conducted after material production, not during the design stage. One researcher stated, “In many cases, we think about performance first. Safety and environmental impact are discussed later, especially when we prepare publication or institutional reports” (P1). This pattern shows that the safe and sustainable by design principle has not been fully embedded in daily laboratory practice. It also suggests the need for a more integrated framework that connects green chemistry, data recording, toxicity assessment, and sustainability indicators from the beginning of research.

The sixth theme shows that the integration of green chemistry and data-driven approaches requires a change in research culture. Participants emphasized that sustainable nanomaterial development cannot rely only on individual researchers. It requires shared standards, institutional data systems, laboratory training, interdisciplinary collaboration, and stronger awareness of environmental responsibility. The study found that researchers who had access to collaborative networks and better documentation systems were more prepared to adopt data-driven approaches. In contrast, laboratories with fragmented records and limited equipment faced greater difficulties in implementing systematic optimization. One participant explained, “The challenge is not only the method, but the habit. We need to record data better, share data more openly, and think about sustainability from the beginning” (P9). This finding shows that sustainable nanomaterial development depends on both technical capacity and research culture.

Discussion

The findings indicate that green chemistry is understood by participants as both a scientific method and an ethical orientation in nanomaterial development. This finding supports Gupta et al. (2023), who argue that green nanomaterial synthesis emerged as a response to the environmental limitations of conventional synthesis methods. It also aligns with Ying et al. (2022), who emphasize the potential of plants, microorganisms, and biomolecules as safer reducing and stabilizing agents. However, this study adds a qualitative perspective by showing that researchers do not experience green chemistry only as a set of technical principles. They also experience it as a responsibility to reduce waste, use local resources, and make laboratory practice more environmentally accountable. This meaning is important because the success of green chemistry depends not only on available materials, but also on how researchers interpret and apply sustainability values in everyday scientific work.

The issue of reproducibility emerged as one of the strongest findings. Participants reported that natural materials provide environmental benefits, but they also create uncertainty because their composition can vary across sources, seasons, and preparation methods. This finding is consistent with Dikshit et al. (2021), who note that green synthesis has practical value but still faces limitations in process control and standardization. Mulyana et al. (2024) also show that the concentration and pH of natural bioreductants can affect the synthesis of silver nanoparticles. The present study extends these findings by showing how reproducibility problems are experienced at the laboratory level. Researchers must negotiate between the desire to use safer local materials and the need to produce stable, predictable, and publishable results. This tension explains why green synthesis requires stronger documentation and analytical support.

The findings also show that data-driven approaches can reduce trial-and-error practices in nanomaterial synthesis. Participants viewed experimental data as a resource for improving decision-making, especially in selecting synthesis parameters and predicting material characteristics. This finding supports Jia et al. (2021), who argue that machine learning can accelerate nanomaterial design and discovery. It also aligns with Kumar et al. (2021), who demonstrate the use of machine learning in selecting sustainable solvents for material synthesis. Ye et al. (2025) further show that machine learning can optimize green synthesis parameters and improve adsorption performance. However, this study finds that the main barrier is not only access to computational tools. The deeper problem lies in fragmented data recording, limited data quality, and the lack of a shared culture of data reuse. This finding offers a new perspective by placing data-driven nanomaterial development within the social and organizational context of laboratory practice.

The study also highlights the importance of nanomaterial databases and FAIR data principles. Participants stated that many experimental results were available, but they were scattered across notebooks, personal files, and unpublished reports. This finding supports Ji et al. (2021), who emphasize the importance of nanomaterial databases for design and risk assessment. Furxhi et al. (2023) also argue that structured and reusable data can support intrinsic hazard assessment in nanomaterial development. The present study strengthens this argument by showing that data quality is shaped by daily research habits. When failed experiments are not documented, when data formats differ across researchers, and when records are not integrated, laboratories lose valuable knowledge that could support future optimization. Therefore, data-driven research requires not only algorithms, but also data discipline, institutional infrastructure, and clear documentation standards.

Another important finding concerns the limited integration of safety and sustainability assessment at the early stage of material design. Participants reported that performance indicators often receive more attention than toxicity, life-cycle impact, and waste management. This finding is relevant to the safe and sustainable by design framework discussed by Furxhi et al. (2022). It also aligns with Chatzipanagiotou et al. (2025), who show that the implementation of safe and sustainable by design remains challenging because of differences in assessment tools, data requirements, and functional unit definitions. This study adds that the challenge is not only methodological, but also cultural. In laboratory practice, safety and sustainability may become secondary concerns when publication pressure, instrument access, and performance targets dominate research priorities. This condition suggests that sustainable nanomaterial development requires earlier integration of risk assessment, not only evaluation after synthesis.

The findings also support the argument that machine learning and nanoinformatics can contribute to safer and more sustainable nanomaterial development. Tripathy et al. (2024) describe the convergence of nanotechnology and machine learning as an opportunity to support synthesis, characterization, and optimization. Xiao et al. (2025) also show that machine learning can assist in evaluating the biological safety and sustainability of metal nanomaterials. Saha (2025) further emphasizes that nanoinformatics can support safer material design through large-scale data. However, the present study shows that the adoption of these approaches depends on researcher capacity, interdisciplinary collaboration, and institutional readiness. Machine learning cannot function effectively if laboratories lack sufficient datasets, standardized records, and researchers who can interpret both chemical and computational results. This means that data-driven sustainability requires human capacity development as much as technological adoption.

From a theoretical perspective, this study contributes to the understanding of sustainable nanomaterial development as a socio-technical process. Green chemistry provides the normative foundation for safer and more efficient synthesis, while data-driven approaches provide analytical support for optimization and prediction. However, both approaches depend on researcher interpretation, institutional practices, laboratory culture, and the availability of reliable data. This finding expands previous technical and review-based studies by showing how sustainability is constructed through everyday decisions in the laboratory. The integration of green chemistry and data-driven approaches is therefore not a linear process. It involves negotiation among safety, material performance, environmental responsibility, data availability, publication demands, and institutional constraints.

From a practical perspective, the findings suggest that laboratories need to develop more systematic data management systems for nanomaterial research. Research teams should record both successful and failed experiments, standardize data formats, document material sources, and include sustainability indicators in laboratory protocols. Institutions also need to support training in green chemistry, nanoinformatics, and basic machine learning for researchers and postgraduate students. Collaboration between chemists, material scientists, data scientists, and environmental experts should be strengthened so that sustainable nanomaterial development can move beyond individual experimentation. These practical steps can help reduce repeated trials, improve reproducibility, and support safer material design.

Future research should examine this issue in a wider range of laboratory settings, including industrial research centers, government laboratories, and interdisciplinary nanotechnology programs. Comparative studies may explore differences between laboratories that already use integrated data systems and those that still rely on conventional documentation. Further research may also combine qualitative interviews with bibliometric analysis, laboratory ethnography, or mixed-method approaches to understand the relationship between research culture, data infrastructure, and sustainable material innovation. In addition, future studies can develop a practical framework for integrating green chemistry indicators, experimental databases, machine learning workflows, and safe and sustainable by design principles in nanomaterial research. Such studies would deepen understanding of how sustainable nanotechnology can be implemented in both scientific and institutional practice.

4. Conclusions

This study concludes that the integration of green chemistry and a data-driven approach in sustainable nanomaterial development is not only a technical process, but also a socio-scientific practice shaped by laboratory culture, data habits, resource availability, and researchers' interpretation of sustainability. The findings show that researchers understand green chemistry as a form of laboratory responsibility that includes safer material selection, waste reduction, energy efficiency, and the use of local biological resources. However, the implementation of green synthesis still faces challenges related to reproducibility, variation in natural materials, fragmented experimental data, limited data infrastructure, and the uneven adoption of machine learning or computational tools. These findings contribute to the literature by showing that sustainable nanomaterial development depends on the interaction between scientific principles, data literacy, safety awareness, and institutional research practices.

The study has theoretical, practical, and policy implications. Theoretically, it expands the understanding of sustainable nanomaterial development as a socio-technical process that combines green chemistry, data-driven decision-making, and safe and sustainable by design principles. Practically, the findings suggest that laboratories need to strengthen data documentation, record both successful and failed experiments, standardize synthesis protocols, and develop interdisciplinary collaboration between material scientists, chemists, data scientists, and environmental experts. From a policy perspective, institutions should support laboratory data systems, training in nanoinformatics and green chemistry, and sustainability assessment guidelines for nanomaterial research. Future studies should examine broader laboratory settings, compare academic and industrial research practices, and develop practical frameworks that integrate green chemistry indicators, experimental databases, machine learning workflows, and safety assessment in sustainable nanomaterial development.

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