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Scientists' Experiences, Trust, and Meaning in AI-Assisted Drug Design

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ABSTRACT

Artificial intelligence has increasingly transformed medicinal chemistry by enhancing the efficiency and scope of drug design processes. However, little is known about how medicinal chemists experience and interpret the integration of AI in their daily research practices. This study explores how medicinal chemists construct meaning, trust, and professional judgment when using AI in drug design. Using an interpretive phenomenological approach, data were collected through semi-structured interviews with medicinal chemistry professionals and analyzed using Interpretative Phenomenological Analysis (IPA). The findings indicate that AI is experienced both as a tool that accelerates molecular exploration and as a source of epistemic tension that requires ongoing human interpretation. While AI expands scientific imagination and supports decision-making, it also raises challenges related to trust and interpretability. Participants described their evolving role as evaluators and interpreters of AI-generated outputs. This study contributes to the understanding of human–AI interaction in medicinal chemistry by highlighting the importance of combining technological advancement with human-centered interpretation to support responsible drug discovery.

INTRODUCTION

The rapid advancement of artificial intelligence (AI) has significantly transformed the landscape of scientific research, particularly within the hfield of medicinal chemistry. Traditionally, drug discovery has been characterized by iterative experimental processes, extensive laboratory validation, and reliance on expert intuition to guide molecular design and optimization. However, the integration of AI and machine learning into medicinal chemistry has introduced new paradigms in which computational systems can generate, predict, and prioritize potential drug candidates with unprecedented speed and efficiency (Moukha-Chafiq et al., 2025). These developments have reshaped how chemical space is explored and how early-stage drug design decisions are made, positioning AI as a central component in contemporary pharmaceutical research environments.

Despite these technological advancements, the increasing reliance on AI has also introduced complex human-centered challenges that extend beyond technical performance. The interaction between scientists and AI systems is not purely mechanical but is embedded within cognitive, epistemological, and professional dimensions of scientific practice. Researchers are required to interpret algorithmic outputs, reconcile them with established chemical knowledge, and make critical decisions under conditions of uncertainty (Kim et al., 2025). This dynamic creates a unique experiential context in which the role of human judgment remains central, even as computational tools become more sophisticated. In this sense, AI in medicinal chemistry is not only a technological innovation but also a phenomenon that reshapes how scientists experience their work, construct meaning, and engage with knowledge production.

The relevance of this phenomenon becomes particularly evident when considering the subjective dimension of scientific practice. While existing literature has extensively examined the technical capabilities of AI in drug discovery, including predictive accuracy and algorithmic efficiency, far less attention has been given to how researchers themselves experience the integration of these technologies into their workflows (Huang et al., 2025). The adoption of AI introduces new forms of cognitive tension, such as negotiating trust in opaque systems, adapting to accelerated decision-making processes, and redefining professional identity in an increasingly data-driven environment. These experiences are deeply embedded in the social and professional contexts in which medicinal chemists operate, making them essential for understanding the broader implications of AI integration.

Given this context, there is a clear need to explore the phenomenon from a perspective that prioritizes lived experience and subjective meaning. A phenomenological approach provides a suitable framework for such exploration, as it seeks to understand how individuals interpret and make sense of their experiences within a particular context (Cocetta et al., 2023). Rather than focusing solely on technological outcomes, this approach allows for a deeper investigation into how scientists perceive, negotiate, and internalize the presence of AI in their research practices. By examining these experiences, the study contributes to a more comprehensive understanding of the human dimension of technological transformation in medicinal chemistry, highlighting the importance of meaning-making processes in shaping scientific knowledge and practice.

Research on the lived experiences of professionals interacting with emerging technologies has increasingly gained attention across scientific disciplines, particularly in contexts where human judgment intersects with algorithmic decision-making. Within medicinal chemistry, this line of inquiry is becoming especially relevant as AI-driven systems are progressively integrated into drug discovery workflows (Chung et al., 2025). While earlier studies have primarily focused on optimizing computational performance and improving predictive models, a growing body of interdisciplinary research has begun to recognize that the subjective experience of researchers plays a critical role in shaping how these technologies are adopted, interpreted, and utilized in practice (Mukhlis, Suradi, et al., 2023; Mukhlis, 2025b). Understanding how scientists experience AI not only as a tool but as an active influence on reasoning, decision-making, and professional identity has therefore emerged as an important area of investigation.

However, exploring such experiences presents significant methodological challenges. The complexity of human-AI interaction in scientific environments involves not only observable behaviors but also internal processes such as interpretation, doubt, trust, and epistemic negotiation (Bist et al., 2025). Conventional research approaches, particularly those grounded in quantitative methods, often rely on measurable indicators such as model accuracy, efficiency, or user satisfaction scores. While these approaches provide valuable insights into system performance, they remain limited in their ability to capture the depth, nuance, and contextual meaning of researchers' lived experiences. As noted in prior studies, the reliance on computational metrics and large-scale data analysis tends to overlook how individuals make sense of AI outputs in relation to their own expertise and professional responsibilities.

These limitations highlight a critical gap in methodological alignment between the nature of the phenomenon and the approaches used to study it (Garvey et al., 2024). The phenomenon of AI integration in medicinal chemistry is inherently experiential, interpretive, and context-dependent, yet much of the existing research treats it as a technical problem rather than a human-centered process. As a result, previous methods have been insufficient in uncovering the essential structure of the experience, particularly in terms of how scientists negotiate meaning, reconcile uncertainty, and redefine their roles in AI-mediated environments (Garde et al., 2025). This inadequacy underscores the need for methodological approaches capable of accessing the depth of subjective experience, thereby enabling a more comprehensive understanding of the phenomenon beyond its measurable dimensions.

In response to the growing integration of artificial intelligence in medicinal chemistry, prevailing approaches to understanding this phenomenon have largely relied on practical and performance-oriented frameworks. Most existing studies emphasize computational efficiency, predictive accuracy, and algorithmic optimization as primary indicators of success in AI-assisted drug discovery. These approaches have contributed significantly to advancing the technical capabilities of AI systems and have provided a foundation for their widespread adoption in pharmaceutical research. Within this dominant paradigm, the interaction between scientists and AI is often treated as a functional relationship, where the human role is reduced to operating, validating, or implementing algorithmic outputs.

However, such approaches remain limited in their ability to capture the deeper experiential and interpretive dimensions of this interaction (Gange et al., 2022). By focusing predominantly on measurable outcomes, prior studies tend to overlook how scientists actually experience the use of AI in their daily research practices. Important aspects such as the negotiation of trust, the emergence of cognitive tension, the reinterpretation of expertise, and the subjective meaning assigned to AI-generated results are often underexplored or entirely absent from the analysis. As a consequence, the current body of knowledge provides an incomplete understanding of the phenomenon, as it fails to address how AI is internalized, interpreted, and navigated within the lived realities of medicinal chemists (Mukhlis, Arifin, Ridwan, & Zulbaidah, 2025; Mukhlis, Arifin, Ridwan, Zulbaidah, et al., 2025). This gap suggests that the existing solutions, while technically robust, do not fully engage with the human dimension that is central to scientific decision-making.

Given these limitations, there is a clear need for an alternative approach that can access the depth and richness of subjective experience. A phenomenological perspective offers a compelling solution, as it is specifically designed to explore how individuals make sense of complex phenomena within their own contexts (Dardas et al., 2025). By focusing on lived experience, phenomenology allows for the identification of essential meanings, interpretive processes, and contextual influences that remain inaccessible through conventional quantitative or performance-based methods. In the context of medicinal chemistry, such an approach enables a more holistic understanding of how AI is experienced not only as a technological tool but also as a transformative element in scientific practice. This shift in perspective is essential for addressing the current knowledge gap and for developing a more comprehensive account of human-AI interaction in drug discovery.

Previous studies have explored patient experiences in healthcare, particularly in relation to treatment adherence, perceived safety, and therapeutic outcomes. Within the domain of drug delivery systems, research has predominantly emphasized clinical effectiveness, pharmacokinetics, and technological innovation, while comparatively fewer studies have examined how patients experience these systems in their everyday lives. Existing qualitative evidence suggests that patient perception, trust in healthcare providers, and emotional responses significantly influence treatment acceptance. In the context of pregnancy, the literature further indicates that women often interpret medical interventions through the lens of maternal responsibility and fetal safety, shaping their decision-making processes in complex and deeply personal ways. However, these studies remain limited in their ability to capture the depth and richness of lived experience, particularly in relation to non-invasive drug delivery systems.

To address this limitation, this study adopts an interpretive phenomenological approach to explore the lived experiences of pregnant women in accepting non-invasive drug delivery systems. This approach is particularly suitable because it enables an in-depth examination of how individuals interpret, negotiate, and assign meaning to their experiences within a specific socio-medical context. By focusing on lived experience, the study seeks to uncover how perceptions of safety, comfort, trust, and integration into daily life influence treatment acceptance. In doing so, the study moves beyond outcome-based and technologically driven evaluations, offering a richer and more nuanced understanding of patient experience. This approach directly responds to the identified knowledge gap by foregrounding subjective meaning as a central component of healthcare decision-making during pregnancy.

This article is structured to provide a coherent and systematic exploration of the phenomenon. The introduction outlines the general and specific background, followed by the identification of the knowledge gap and the rationale for the study. The method section details the phenomenological design, participant characteristics, data collection procedures, and analytical framework (Mukhlis et al., 2024; Mukhlis, Maryam, et al., 2023). The results section presents the key themes derived from participants' lived experiences, supported by illustrative quotations. The discussion interprets these findings in relation to existing literature, and the conclusion highlights the theoretical and practical implications for future research on human-AI interaction in medicinal chemistry and AI-assisted drug discovery practice.

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RESEARCH METHODS

Study Design

A phenomenological design was employed to examine the lived experience of scientists using artificial intelligence in medicinal chemistry, particularly in the context of drug design. This approach was considered appropriate because the research question centered on subjective meaning, professional judgment, and the interpretive processes through which scientists engaged with AI-generated outputs (Lutz & Knox, 2014; McNabb, 2015). Rather than measuring technological performance or computational accuracy, the study focused on how the phenomenon was experienced, understood, and negotiated within the participants' everyday scientific practice.

An interpretative phenomenological orientation was adopted to capture both the immediacy of participants' accounts and the deeper meanings embedded in those accounts. This approach is especially suitable when a phenomenon involves complex cognition, professional identity, and reflective sense-making, as it allows careful attention to how individuals interpret their own experience within a particular context. In the present study, the phenomenon was not treated as a purely technical event, but as a situated human experience shaped by scientific responsibility, epistemic uncertainty, and technological interaction. The design therefore enabled an in-depth exploration of how medicinal chemistry researchers perceived AI as a tool, a challenge, and a transformative presence in their research workflow. The study was conducted after obtaining ethical approval from the relevant institutional ethics committee, and all participants provided informed consent before taking part in the interviews. Confidentiality, voluntary participation, and the right to withdraw from the study were clearly explained to each participant.

Participants

Participants consisted of professionals working in fields closely related to medicinal chemistry and AI-assisted drug design. Eligibility was defined through purposive criteria to ensure that all participants had direct and meaningful experience with the phenomenon under investigation. Inclusion criteria comprised active involvement in medicinal chemistry research, computational drug design, cheminformatics, pharmaceutical R&D, or related translational research settings; practical experience using AI or machine learning tools in molecular screening, candidate prioritization, or structure-based decision-making; and the ability to reflect critically on that experience in an interview setting. Participants were required to have at least one year of relevant professional exposure in order to ensure sufficient familiarity with both the scientific process and the use of AI-supported systems.

Exclusion criteria included individuals whose knowledge of AI in medicinal chemistry was limited to theoretical exposure without actual application, researchers working exclusively in unrelated laboratory domains, and participants who could not provide sufficiently detailed experiential accounts. A purposive sampling strategy was used to identify information-rich cases capable of illuminating the phenomenon in depth (Hillman & Radel, 2018; Migdal, 2018). This strategy is widely aligned with phenomenological inquiry because it privileges experiential relevance over numerical representativeness.

A small and focused sample was considered appropriate in accordance with interpretative phenomenological research principles, which emphasize depth rather than breadth. The participant group may be described in the final manuscript using relevant demographic and professional characteristics such as number of participants, gender distribution, age range, academic qualification, years of experience, institutional affiliation, and primary area of specialization. These contextual details are important because the experience of AI in medicinal chemistry may be shaped by disciplinary training, level of seniority, and degree of exposure to computational methods.

Data Collection

Data were collected through in-depth semi-structured interviews designed to elicit detailed descriptions of participants' lived experiences with AI in medicinal chemistry. A semi-structured interview format was selected because it provided sufficient consistency across interviews while also allowing flexibility for participants to elaborate on meanings, tensions, and reflections that emerged naturally during conversation (Carreiras & Castro, 2012; Iosifides, 2016). The interview guide was developed around key areas relevant to the research question, including first encounters with AI tools, perceived benefits and limitations, trust in algorithmic outputs, tensions between computational predictions and chemical intuition, and the perceived impact of AI on scientific identity and decision-making.

Interviews were conducted individually in a setting that ensured privacy, minimal interruption, and psychological comfort. Depending on participant availability and institutional context, interviews could be conducted either face-to-face or through secure online meeting platforms. Each interview was expected to last approximately 45 to 90 minutes, allowing adequate time for narrative depth without imposing excessive burden on participants. With consent, all interviews were audio-recorded and later transcribed verbatim to preserve the integrity of participants' expressions. Field notes were also prepared during or immediately after the interviews to document contextual cues, nonverbal observations when available, and preliminary experiential impressions relevant to interpretation.

The interview process was conducted in a manner intended to support openness and reflective depth. Participants were encouraged to describe concrete moments, professional dilemmas, and personal responses rather than provide only abstract evaluations of AI. Follow-up prompts were used to clarify meaning, deepen description, and explore the context surrounding specific experiences. Data collection continued until sufficient experiential depth and thematic richness had been achieved, with attention given to the recurrence of interpretively meaningful patterns across accounts rather than to numerical saturation in a purely positivist sense.

Data Analysis

Data were analyzed using Interpretative Phenomenological Analysis (IPA), an approach well suited to exploring how participants make sense of complex and professionally significant experiences. This analytical framework was chosen because the study aimed not only to document what participants experienced, but also to understand how those experiences were interpreted in relation to scientific responsibility, trust, expertise, and technological change.

Analysis proceeded through a systematic multi-stage process. First, each transcript was read repeatedly to facilitate immersion in the data and to preserve the idiographic focus of each participant's account. Initial notes were then developed by attending to descriptive content, linguistic expression, and conceptual significance (Daly, 2007; Longhofer et al., 2012). These notes were used to identify emergent meaning units grounded in participants' own words while remaining sensitive to interpretive depth. In the next stage, closely related meaning units were clustered into preliminary themes within each case. Attention was then directed to patterns of convergence and divergence across cases in order to develop higher-order thematic structures that captured the shared essence of the phenomenon without erasing individual nuance.

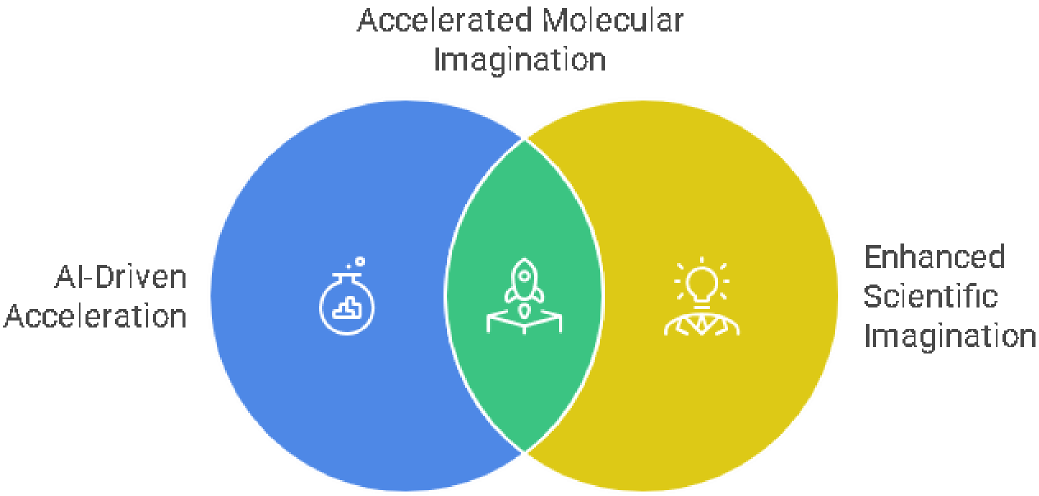
The analysis remained iterative throughout. Earlier interpretations were revisited in light of later transcripts, and developing themes were refined through repeated comparison with the original data. The resulting thematic structure was designed to reflect both the participants' lived experience and the interpretive complexity of engaging with AI in medicinal chemistry. Qualitative data management software such as NVivo may be used to support transcript organization, coding traceability, and retrieval of theme-linked excerpts, although interpretive judgment remained central to the analysis (Fife, 2020; Kawamura, 2020). This analytic process enabled the emergence of essential findings concerning acceleration, trust, epistemic tension, and the redefinition of scientific roles in AI-mediated research environments.

RESULTS

Encountering AI as an Accelerator of Molecular Imagination

Participants consistently described AI as expanding the speed and breadth of early-stage molecular exploration. The technology was experienced as a system that rapidly opened new chemical possibilities that would otherwise require extensive time, repeated manual reasoning, and iterative computational screening. For several participants, AI changed the rhythm of scientific work by allowing them to move more quickly from conceptual uncertainty to candidate generation. This acceleration, however, was not experienced merely as convenience; it was often narrated as a transformation in how scientific imagination itself was mobilized.

The Synergy of AI and Scientific Imagination



One participant explained that AI made the ideation process feel broader and less constrained by habitual reasoning: "Before using AI, I tended to think within familiar scaffolds and known structural logic. With AI, I suddenly saw molecular suggestions that I would not have manually prioritized, and that changed how I imagined the chemical space." This account suggests that AI functioned not only as a predictive instrument but also as a catalyst for reframing the boundaries of what was scientifically thinkable.

Another participant similarly described AI as enabling a more exploratory mindset: "It gave me options much faster than my usual workflow. I felt as if I was not starting from zero anymore. The system offered directions, and I could immediately begin judging them rather than spending days constructing them manually." In this sense, participants experienced AI as reducing the burden of initial search and allowing more energy to be directed toward evaluation and refinement.

Yet this acceleration was not interpreted as simple liberation. Some participants described the speed of AI-generated outputs as overwhelming, especially when the number of candidate molecules exceeded what could be meaningfully reviewed within the practical limits of laboratory reasoning. A participant noted, "The system can generate many promising compounds, but that abundance creates another challenge. You start asking yourself whether faster generation really means better understanding." This indicates that acceleration was accompanied by a sense of intellectual compression, where scientific reasoning had to keep pace with the rapidly expanding field of possibilities.

Across interviews, AI was therefore experienced as an accelerator of molecular imagination, but not in a purely celebratory sense. It widened the horizon of drug design while simultaneously confronting researchers with the need to manage abundance, prioritize possibilities, and preserve interpretive depth in the face of computational speed.

Negotiating Trust Under Conditions of Opacity

A central feature of participants' experience was the ongoing negotiation of trust. Although AI-generated results were often regarded as impressive and potentially useful, they were rarely accepted without hesitation. Participants repeatedly emphasized that the predictive power of AI did not automatically produce epistemic confidence. Instead, trust emerged as conditional, fragile, and deeply tied to the perceived transparency of the model.

Many participants described a persistent unease regarding the "black box" nature of AI systems. One participant stated, "The prediction may be statistically strong, but if I do not understand why the model prefers one structure over another, I cannot fully trust it as a scientist." This statement reflects a distinction between performance and intelligibility. For participants, scientific confidence was not based solely on output quality, but also on the ability to situate that output within an understandable chain of reasoning.

Another participant described trust as something that had to be earned through repeated verification: "I never use AI output as a final answer. I treat it as a suggestion that must pass through my own chemical logic, literature checks, and sometimes biological plausibility before I consider it credible." This shows that trust was experienced as procedural rather than immediate. AI recommendations entered the workflow as provisional propositions that required human validation before being integrated into scientific decision-making.

For some participants, trust was further shaped by prior experiences of model inconsistency. One participant reflected, "Sometimes the model identifies compounds that look highly promising computationally, but when you examine them more deeply, they are chemically impractical or biologically unrealistic. After that, you become more cautious." Such experiences created a cautious posture in which AI remained useful but never fully autonomous in the research process.

Importantly, participants did not reject AI because of opacity. Rather, they developed adaptive strategies for working with partial trust. These strategies included cross-validating results with known medicinal chemistry principles, consulting colleagues, comparing AI suggestions with prior literature, and manually interrogating structural plausibility. In this way, trust was experienced as dynamic and negotiated rather than granted. AI entered the workflow as an influential but not fully transparent partner, one whose value depended on continuous human scrutiny.

Experiencing Epistemic Tension Between Computational Prediction and Scientific Judgment

Beyond questions of trust, participants described a deeper tension concerning the status of scientific judgment itself. AI predictions were often experienced as intellectually provocative because they could challenge established reasoning patterns, propose unexpected molecular candidates, or prioritize compounds that contradicted intuitive expert expectations. This generated a recurrent epistemic tension between what the system predicted and what the scientist felt able to justify.

One participant articulated this tension clearly: "There were times when the AI ranked a molecule very highly, but chemically I felt unconvinced. In those moments, I had to decide whether I should trust the algorithm or trust the instincts built from years of medicinal chemistry work." This quotation captures the lived conflict between data-driven recommendation and embodied expertise. The tension was not simply methodological; it was existentially tied to participants' identities as scientists trained to reason through mechanism, structure, and pharmacological plausibility.

Another participant explained that AI sometimes forced a reconsideration of what counts as evidence in drug design: "I realized that my discomfort was not only about the model. It was also about me having to redefine what I consider convincing evidence when a machine presents a result before I fully understand the rationale." This suggests that AI was experienced as a disruptive epistemic presence, requiring participants to renegotiate their own standards of certainty and justification.

Some participants described this tension as productive. Rather than viewing disagreement between AI and expert reasoning as a problem, they saw it as an opportunity for critical reflection. One participant noted, "The most valuable moments were actually when I disagreed with the AI. That forced me to explain my assumptions more carefully and sometimes revealed that my intuition was too conservative." Here, AI functioned as a stimulus for reflexivity, prompting participants to examine the foundations of their own decision-making.

Nevertheless, the tension was not always experienced positively. For others, repeated divergence between computational output and scientific intuition produced frustration and cognitive fatigue. A participant reported, "You spend a lot of time trying to reconcile two worlds—the computational ranking and your own chemical reasoning and that process can be mentally exhausting."

Thus, the experience of AI in medicinal chemistry was marked by an ongoing effort to reconcile predictive efficiency with interpretive accountability.

Taken together, these accounts show that participants did not experience AI as replacing judgment, but as intensifying the need to articulate, defend, and sometimes revise scientific judgment. The phenomenon was not one of passive adoption, but of constant epistemic negotiation.

Redefining the Role of the Medicinal Chemist in an AI-Mediated Environment

Participants also described AI as transforming how they understood their own professional role. Rather than seeing themselves solely as designers of molecules, they increasingly experienced their work as involving interpretation, filtration, ethical restraint, and the translation of computational output into scientifically meaningful action. The presence of AI appeared to redistribute, rather than eliminate, human agency within medicinal chemistry.

One participant explained this shift as follows: “I no longer feel that my role is to manually generate every possibility. My role now is to interrogate, select, and contextualize what the system proposes.” This reflects a movement from direct construction toward evaluative stewardship. The medicinal chemist was experienced less as a solitary originator of molecular ideas and more as a critical mediator between algorithmic possibility and scientific relevance.

Another participant described this redefinition in terms of responsibility: “AI can recommend structures, but it does not carry responsibility for poor scientific decisions. That responsibility stays with us. So in a way, the human role becomes even more important, not less.” This statement highlights that participants experienced AI not as a transfer of accountability, but as a condition that heightened the ethical and intellectual obligations of the researcher.

Several participants also reported that AI required new competencies beyond traditional medicinal chemistry expertise. These included the ability to interpret model outputs, identify algorithmic limitations, communicate across interdisciplinary teams, and remain reflective about technological influence on scientific decisions. One participant stated, “Using AI effectively is not just about chemistry anymore. It also requires understanding what the model can and cannot tell you, and that changes the profile of the researcher.” The role of the medicinal chemist was therefore experienced as expanding into a more hybrid form of expertise.

At the same time, participants resisted the idea that AI diminished the value of human intuition. Instead, they described intuition as being repositioned. A participant expressed this by saying, “My intuition still matters, but it works differently now. It is less about guessing the next molecule and more about judging whether the machine’s suggestion makes scientific sense.” This indicates that the emergence of AI did not erase expert subjectivity, but transformed its function within the research process.

Overall, participants experienced AI as reshaping professional identity in medicinal chemistry. The scientist became a validator, interpreter, and epistemic gatekeeper, responsible for preserving meaning, plausibility, and accountability within an increasingly AI-mediated workflow.

DISCUSSION

The findings indicate that the use of artificial intelligence in medicinal chemistry is experienced not merely as a technical enhancement, but as an interpretive and professional reorientation in which acceleration, opacity, epistemic tension, and role transformation are lived simultaneously. In relation to the broader question raised in the Introduction, the study shows that the meaning of AI in drug design lies not only in what it can predict, but in how scientists experience, evaluate, and negotiate its presence within knowledge production.

This study contributes to the research question by clarifying that the subjective experience of AI in medicinal chemistry is structured by a persistent tension between computational possibility and human responsibility (Cunha Reis, 2025). The Results showed that participants did not experience AI as a neutral or self-sufficient instrument. Instead, they described it as an influential system that

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broadened molecular imagination while simultaneously requiring caution, interpretation, and professional restraint. This is an important contribution because it moves the discussion beyond a functional account of AI adoption and demonstrates that the real significance of AI in medicinal chemistry emerges through lived engagement. In other words, the phenomenon is not exhausted by speed, prediction, or optimization; it is constituted through the scientist's effort to render computational output meaningful, credible, and scientifically defensible.

The first contribution of these findings lies in showing that acceleration is not experienced as an unqualified benefit. Existing discourse often presents AI as valuable because it shortens timelines and expands the searchable chemical space, which is indeed a major promise of machine learning in drug discovery. Yet the present findings add a phenomenological layer to that promise by revealing that acceleration can also produce interpretive burden (Cheung & Barrett, 2023). When participants described AI as opening many molecular possibilities at once, they also described the need to manage abundance, ambiguity, and the pressure to decide responsibly (Mukhlis, Janwari, et al., 2023; Mukhlis & Abdullah, 2025). This means that computational speed does not eliminate human work; rather, it redistributes that work toward evaluation, prioritization, and justification. The lived meaning of acceleration, therefore, is ambivalent: it is experienced as both empowerment and compression. This nuanced insight helps answer the research question by showing that scientists' experiences with AI are shaped not only by efficiency gains but also by the practical and cognitive consequences of those gains.

A second contribution concerns trust. The findings suggest that trust in AI is not immediate, binary, or purely determined by predictive performance. Instead, trust is procedural and negotiated. Participants repeatedly described the need to verify AI-generated suggestions against chemical plausibility, literature knowledge, and their own professional reasoning (Chambal et al., 2023). This is significant because it shows that trust in scientific AI is relational and interpretive rather than automatic. The opacity of many AI models appears to intensify this condition. Even when outputs are promising, participants experienced uncertainty if the rationale behind a prediction could not be understood in a way consistent with scientific reasoning. Thus, the study answers the research question by showing that the subjective experience of AI is inseparable from the moral and epistemic responsibility of deciding when an output is sufficiently intelligible to be used. In this context, trust becomes less a matter of confidence in technology alone and more a matter of how scientists preserve accountability while working with partially explainable systems.

A third contribution is the identification of epistemic tension as a central experiential structure. Participants did not simply compare their own judgment with AI output; they experienced moments in which their scientific identity and standards of evidence were challenged by the machine's recommendations. This is especially important because it reveals that AI use in medicinal chemistry is not only operational but epistemological (Ben-Zeev et al., 2024). The scientists in this study were compelled to confront questions such as what counts as convincing evidence, how much weight should be assigned to algorithmic ranking, and when intuition should yield to prediction. The study therefore contributes a deeper understanding of how AI reshapes scientific reasoning from within. Rather than replacing expert judgment, AI appears to intensify the visibility of judgment by forcing scientists to articulate, defend, and sometimes revise their assumptions. This insight directly addresses the research question by demonstrating that the lived experience of AI is characterized by active negotiation rather than passive acceptance.

The fourth contribution concerns professional identity. The findings suggest that AI changes the role of the medicinal chemist from being primarily a generator of candidate ideas to becoming an interpreter, curator, and epistemic gatekeeper of computational possibilities. This role transformation is highly relevant because it indicates that AI integration does not diminish the need for expertise; rather, it reconfigures expertise. Participants' accounts show that scientific authority now depends not only on chemical knowledge, but also on the ability to critically interrogate model outputs, detect limitations, and contextualize computational suggestions within biological and practical reality. The study thus contributes a more human-centered understanding of AI adoption, one in which technology does not displace the scientist but changes the form through which scientific responsibility is enacted.

These findings are broadly consistent with prior literature showing that machine learning has become increasingly influential across multiple stages of drug discovery, especially in target identification, screening, and decision support. Reviews by Vamathevan et al. emphasize that machine learning can improve data-driven decision-making in drug discovery, while Zhavoronkov and colleagues similarly frame AI as a transformative force with the potential to accelerate pharmaceutical research (Babawo et al., 2025). The present study supports those claims, particularly in relation to speed, expanded search capacity, and the reframing of early-stage scientific work. However, it extends this literature by showing that acceleration at the system level is experienced by scientists as interpretive complexity at the human level. The literature has convincingly established what AI can do in technical terms; the present findings clarify what it feels like to work with those capabilities in practice.

The findings also complement a growing body of qualitative and interpretive work on human-technology interaction. Prior phenomenological and interpretive scholarship has argued that technology adoption cannot be fully understood through causal or performance-based frameworks alone, because digital systems become entangled with users' lifeworlds, judgments, and ongoing sense-making. In this respect, the present study aligns with the view that interpretive phenomenological analysis is especially useful for examining how people engage with technologies whose meaning exceeds their instrumental function. The current findings illustrate this clearly: AI in medicinal chemistry is not merely used; it is encountered, questioned, negotiated, and integrated into professional self-understanding. This relationship between technology and meaning helps explain why quantitative evaluations of usability or effectiveness, although important, remain insufficient for capturing the full essence of the phenomenon.

At the same time, the findings add nuance to optimistic narratives about AI-assisted science. Much of the literature presents AI as a tool for better prediction and faster innovation, and that position is not contradicted here. What this study suggests, however, is that scientific adoption is mediated by interpretive labor. The outputs of AI do not become scientifically actionable merely because they are generated; they become actionable when they are subjected to human scrutiny and incorporated into a meaningful chain of reasoning. In that sense, the present findings neither reject nor romanticize AI. Instead, they reveal that the broader promise of AI in medicinal chemistry depends in part on whether researchers can sustain confidence, accountability, and interpretive control while working with increasingly complex computational systems. This complements earlier technical reviews by foregrounding the human condition of implementation rather than the algorithmic condition of performance.

Viewed more broadly, the study suggests that the essence of the phenomenon lies in the coexistence of possibility and uncertainty. AI expands what scientists can see and generate, but it also makes visible the limits of explanation, the fragility of trust, and the enduring necessity of judgment. This broader interpretation is theoretically important because it places the lived experience of medicinal chemists within a wider conversation about scientific practice in technologically mediated environments. The findings therefore enrich existing literature by demonstrating that the human meaning of AI in drug design cannot be reduced to adoption metrics or performance outcomes alone. Instead, it must be understood as a situated experience in which knowledge, responsibility, and professional identity are continuously renegotiated.

The implications of these findings are both scientific and practical. Scientifically, the study shows that the integration of AI in medicinal chemistry cannot be understood adequately through a purely technical lens. The phenomenon is not limited to computational assistance in molecular prediction, but extends into the lived domain of trust, interpretation, and professional accountability. This means that AI should be viewed not only as an innovation in drug discovery infrastructure, but also as a factor that reshapes how scientific knowledge is produced, judged, and legitimized. In this regard, the present findings deepen the broader arguments advanced in earlier literature, such as Vamathevan et al. and Zhavoronkov et al., by demonstrating that the value of AI in drug discovery is inseparable from the human experience of using it in real research environments.

From a practical perspective, the findings suggest that successful AI integration in medicinal chemistry depends not only on model performance but also on how researchers are supported in interpreting and evaluating AI-generated outputs. The recurring themes of procedural trust, interpretive burden, and epistemic tension indicate that implementation strategies should include more than technical training (Mukhlis, 2025a; Mukhlis & Saidah, 2025). They should also foster critical literacy regarding model limitations, scientific interpretability, and responsible decision-making. In professional settings, this may have implications for the design of interdisciplinary training environments in which medicinal chemists, computational scientists, and pharmaceutical researchers can develop a shared understanding of how AI outputs should be read and used. Such a perspective is especially relevant in contexts where AI systems increasingly influence early-stage candidate selection and research prioritization.

The findings also carry wider social and professional meaning. At a professional level, they indicate that scientific expertise is not diminished by AI but reconfigured by it. The medicinal chemist remains central, although the form of expertise shifts from direct generation toward interpretive selection, contextual evaluation, and responsibility for scientific plausibility. At a broader level, this reflects a wider transformation occurring across knowledge-intensive fields, where emerging technologies do not simply automate practice but alter how professionals understand their own authority, responsibility, and role in decision-making. The present findings therefore speak not only to medicinal chemistry, but also to broader discussions about human agency in technologically mediated scientific work. They are particularly relevant for institutions, laboratories, and research cultures seeking to implement AI while maintaining scientific rigor, accountability, and reflective judgment.

These findings may also be relevant to wider populations beyond the immediate participant group. Although the study focuses on medicinal chemistry, the experiential structure identified here expanded possibility accompanied by uncertainty, caution, and reinterpretation of expertise may resonate with other scientific and clinical domains where AI is becoming embedded in professional reasoning. Researchers in pharmaceutical sciences, computational biology, translational medicine, and related areas may encounter similar tensions when balancing algorithmic output with domain expertise. The contribution of this study, therefore, lies not in claiming universal transferability, but in offering a conceptually rich account that may help illuminate comparable experiences in adjacent settings.

Several limitations should be acknowledged. First, as with most phenomenological studies, the purpose of the research was depth of understanding rather than statistical generalization. The findings therefore illuminate the meaning structure of the phenomenon within a specific experiential and professional context, but they should not be interpreted as representing all medicinal chemists or all scientific encounters with AI. Second, the study is shaped by the contextual specificity of the participants, including their disciplinary background, professional seniority, degree of exposure to AI, and institutional environment. These factors may influence how AI is interpreted and experienced, and the themes identified here may take somewhat different forms in other research settings.

A further limitation concerns the methodological nature of phenomenology itself. Because the study privileges subjective meaning, the findings are necessarily interpretive and context-bound. This is a strength in relation to the research question, but it also means that the analysis does not aim to produce causal claims about AI adoption or to evaluate the objective superiority of particular technologies. In addition, the experience reported by participants may have been shaped by the specific kinds of AI systems they used, including differences in interface design, level of transparency, and degree of integration into the research workflow. As a result, the meanings described here should be understood as grounded in lived experience rather than as exhaustive claims about all AI applications in medicinal chemistry.

These limitations, however, also point toward productive directions for future research. Further studies could examine how the experience of AI differs across subfields of pharmaceutical research, levels of professional experience, or institutional cultures. Comparative phenomenological work could explore whether early-career scientists, senior medicinal chemists, and computational specialists construct trust and professional identity differently when engaging with AI-supported systems. Additional research could also investigate how interpretive experiences evolve over time, particularly as AI becomes more embedded in routine research practice and as scientists become more accustomed to working with algorithmic systems.

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Future work may also expand the present findings by connecting lived experience with broader organizational and educational questions. For example, research could explore how training environments shape the development of trust, how interdisciplinary collaboration affects the interpretation of AI outputs, or how institutional norms influence the balance between computational prediction and expert judgment. Such studies would not replace the value of technical evaluations, but would complement them by clarifying the human conditions under which AI becomes meaningful and usable in scientific practice. In this sense, the present study offers a foundation for a more comprehensive research agenda in which the future of AI in medicinal chemistry is examined not only in terms of performance, but also in terms of experience, meaning, and professional responsibility.

Overall, the study contributes to the field by showing that the significance of AI in medicinal chemistry lies not only in its predictive capabilities, but also in the way it reorganizes the lived experience of scientific work. This insight opens further opportunities for research that integrates technical advancement with human-centered understanding, thereby supporting a more balanced and responsible development of AI in drug discovery.

CONCLUSION

This study examined the lived experience of medicinal chemists in using artificial intelligence within drug design, addressing the need to understand the phenomenon beyond its technical function. The findings reveal that AI is experienced not only as an accelerator of molecular exploration but also as a source of interpretive complexity, where trust, epistemic tension, and professional responsibility become central. The study demonstrates that scientists actively negotiate AI outputs rather than passively adopt them, highlighting the essential role of human judgment in maintaining scientific validity. These results contribute to the existing literature by filling the gap in understanding the subjective and experiential dimensions of AI integration, which have been largely overlooked in performance-oriented research. The findings provide practical value by emphasizing the importance of interpretive competence and responsible decision-making in AI-supported medicinal chemistry workflows. From a practical perspective, the results suggest that the successful implementation of AI-assisted medicinal chemistry requires not only advanced computational tools but also the development of scientists' capabilities to critically evaluate, interpret, and validate AI-generated recommendations. Organizations and research teams should therefore promote training, transparent AI practices, and human-centered decision-making frameworks to ensure the responsible use of AI in drug discovery. This study is not without limitations. The findings are based on the experiences of a specific group of medicinal chemists and may not fully represent the perspectives of researchers from other scientific disciplines, organizational contexts, or levels of AI adoption. In addition, the phenomenological approach prioritizes depth of understanding over generalizability, limiting the extent to which the results can be broadly applied. Future research can expand this work by exploring variations in experience across different scientific domains, levels of expertise, and evolving AI systems to further deepen understanding of human-AI interaction in scientific practice.

CONFLICT OF INTEREST

The authors declare that there is no conflict of interest regarding the publication of this article.

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