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Drivers and Outcomes of Implementing Machine Learning Technology in the Analysis of Experimental Synchrotron Data Using an Interpretive Structural Analysis Approach and Foresight

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Abstract

This study aims to identify and model the drivers and outcomes of implementing machine learning technology in the analysis of experimental synchrotron data using an interpretive structural analysis approach. The research is both applied and exploratory-descriptive in nature, seeking not only to analyze the current state but also to provide a foresight into the future development of the technology and its potential impacts. The participant population consisted of three main groups: theoretical experts (university professors and researchers in technology management), practical experts (executive managers and specialists in machine learning and experimental synchrotron data analysis), and executive managers with at least 10 years of technology management experience. Participants were selected through purposive sampling, reaching theoretical saturation with 10 participants. Data were collected through in-depth interviews and a decision matrix-based questionnaire, and analyzed and coded using qualitative content analysis in MaxQDA software. In the second section, interpretive structural modeling (ISM) and MICMAC analysis were employed to determine relationships among constructs and design the model. Findings indicate that drivers such as the volume of experimental data, expected analysis accuracy, the need for automation of the analysis process, and the development of computational infrastructure have the most influential roles and are positioned as strategic drivers at the top of the model. Additionally, outcomes including enhanced analysis quality and accuracy, reduced processing time, the creation of technological competitive advantages, and the generation of new knowledge fulfill the role of operational and value-creating model outputs. From a foresight perspective, it is predicted that the integration of machine learning technology with experimental synchrotron data analysis will not only enhance the accuracy and speed of analyses but also establish an integrated, data-driven, and scalable process, thereby elevating organizations' capacity for scientific development, innovation, and the creation of sustainable technological advantages. The research results systematically map the logical pathway from technological drivers to operational and value-creating outcomes, providing a foundation for strategic long-term decision-making and planning in the field of synchrotron data analysis.

Keywords: *Machine learning, synchrotron data analysis, interpretive structural modeling, drivers, outcomes*

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1. Introduction

Synchrotron radiation facilities represent pivotal infrastructure for cutting-edge materials science, enabling non-destructive, high-resolution analysis of complex physical, chemical, and biological systems at atomic and molecular scales [1]. The exponential growth in synchrotron data volume—driven by advanced detectors, faster beamlines, and multi-modal imaging techniques—has created unprecedented opportunities for scientific discovery while simultaneously generating formidable analytical challenges [2, 3]. Current data processing pipelines, often reliant on manual or semi-automated methods, struggle to keep pace with the scale, complexity, and multidimensionality of modern synchrotron datasets, leading to bottlenecks in scientific throughput, reproducibility, and the extraction of actionable insights [4, 5]. This critical gap necessitates a paradigm shift toward intelligent, adaptive analytical frameworks capable of transforming raw synchrotron data into high-value scientific knowledge at unprecedented speed and scale.

Machine learning (ML) has emerged as a transformative solution, demonstrating remarkable efficacy in automating data processing, enhancing analytical accuracy, and uncovering latent patterns within synchrotron datasets [6-8]. Recent advancements showcase ML's capacity to revolutionize key synchrotron applications: from real-time beamline optimization [9] and artifact identification in diffraction data [10] to predictive fatigue life modeling of additively manufactured metals [11] and non-targeted metallomics for cancer screening [7]. Notably, ML-driven approaches have enabled breakthroughs in *in situ* and *operando* characterization, allowing researchers to capture dynamic material processes with temporal resolution previously deemed impossible [12, 13]. For instance, the integration of ML with synchrotron X-ray tomography has facilitated the real-time reconstruction and analysis of complex 3D structures, significantly accelerating materials discovery and development cycles [5, 8].

Despite these promising advances, the *systematic implementation* of ML within synchrotron data analysis ecosystems remains fragmented and underdeveloped from a management perspective. Current literature predominantly focuses on technical feasibility and algorithmic performance, often neglecting the critical organizational, strategic, and human dimensions required for sustainable adoption [14, 15]. This oversight creates a significant disconnect between technological potential and practical realization. As highlighted by Karagardimqani et al. [14], successful ML integration demands more than technical proficiency; it requires deliberate strategic alignment, cross-functional collaboration, and adaptive management frameworks capable of navigating the inherent uncertainties of emerging technologies. Similarly, Karkhabad et al. [15] emphasize that ML deployment in complex scientific environments necessitates robust infrastructure planning, change management strategies, and continuous skill development to overcome resistance and ensure long-term value capture.

The management of ML implementation in synchrotron contexts is further complicated by the interdisciplinary nature of the field, where domain experts (materials scientists, physicists), data scientists, and IT specialists must collaborate seamlessly [16, 17]. This complexity is compounded by the rapid evolution of ML methodologies and synchrotron instrumentation, creating a dynamic environment where strategic decisions must balance immediate analytical needs with long-term technological trajectories [18, 19]. Existing frameworks for technology adoption, such as the Technology-Organization-Environment (TOE) framework, often fail to capture the nuanced interplay between *technical capabilities* (e.g., computational infrastructure), *organizational readiness* (e.g., data governance, skill sets), and *environmental pressures* (e.g., funding mandates, competitive research landscapes) specific to synchrotron facilities [20, 21].

Recent studies underscore the critical role of *strategic foresight* in navigating this complexity. Miradi et al. [22] demonstrate how foresight methodologies can proactively identify emerging ML capabilities and their potential impacts on cybersecurity and data integrity in scientific workflows. Similarly, Vizoso and Dingreville [23] advocate for ML-driven tutorials that demystify complex data analysis, enhancing user adoption and reducing the "black box" perception that often hinders technology uptake in scientific communities. However, these studies primarily address technical or educational aspects, leaving a significant gap in *strategic management frameworks* that explicitly map the causal pathways between ML implementation drivers and organizational outcomes within synchrotron contexts.

The literature also reveals a critical tension between *data volume* and *analytical quality*. While larger datasets offer greater potential for ML model training and insight generation [2, 24], they simultaneously amplify challenges in data management, storage, and processing efficiency [3,

4]. This tension is not merely technical; it has profound strategic implications. As Meister et al. [25] observed in early synchrotron ML applications, the absence of scalable computational infrastructure directly constrains the ability to leverage data volume for improved analytical accuracy and innovation. Conversely, the *need for automation* (NAA) and *computational infrastructure development* (CID) emerge as critical enablers, yet their strategic prioritization remains poorly understood [14, 21].

Furthermore, the *outcomes* of ML implementation extend far beyond technical efficiency. Research by Kim et al. [26] demonstrates how ML-enhanced synchrotron analysis can generate *technological competitive advantage* (TCA) through unique analytical capabilities, while Xiang et al. [13] link ML-driven *operando* studies to *new knowledge generation* (GNKT) and theoretical advancements in materials science. However, these outcomes are not automatic; they depend on the strategic orchestration of drivers such as data volume (EDV), expected accuracy (EAA), and infrastructure (CID) [27, 28]. The absence of a clear, evidence-based pathway connecting these drivers to tangible organizational outcomes represents a significant barrier to effective strategic planning.

This gap is particularly acute in the context of *funding and resource allocation*. Synchrotron facilities operate under intense pressure to demonstrate scientific impact and justify substantial capital investments [9, 29]. Without a robust understanding of *how* ML implementation drives specific outcomes—such as accelerated discovery cycles, enhanced analytical quality (IAQ), reduced processing time (RAT), and sustained competitive advantage (TCA)—facility managers lack the evidence needed to prioritize investments and secure future funding [19, 23]. The current reliance on anecdotal evidence or isolated case studies fails to provide the systematic, actionable insights required for strategic decision-making at the organizational level [6, 17].

Theoretical foundations from management science further illuminate this challenge. He and Liu [18] emphasize that the *knowledge evolutionary process* of AI technologies requires deliberate management to transition from isolated applications to integrated strategic assets. Similarly, Miller [21] argues that understanding micromechanical material behavior through synchrotron X-rays necessitates *in situ* management of the analytical workflow, highlighting the need for adaptive, process-oriented leadership. Yet, these insights remain largely unapplied to the specific context of ML-driven synchrotron data analysis.

The convergence of these challenges—technical complexity, interdisciplinary collaboration needs, strategic uncertainty, and the critical need for evidence-based management—creates a compelling case for a dedicated, holistic research focus. This study addresses the critical gap by developing a *comprehensive, foresight-oriented framework* that systematically maps the drivers and outcomes of ML implementation in synchrotron data analysis. Moving beyond purely technical assessments, it integrates management theory with empirical insights from synchrotron practitioners to elucidate the strategic pathways through which ML adoption translates into tangible organizational value. By employing interpretive structural modeling (ISM) and MICMAC analysis, this research identifies the hierarchical relationships between key constructs—such as data volume (EDV), analytical accuracy (EAA), automation needs (NAA), infrastructure development (CID), analytical quality (IAQ), processing time reduction (RAT), competitive advantage (TCA), and knowledge generation (GNKT)—and demonstrates how these elements interact within the complex ecosystem of synchrotron facilities.

This work builds upon and extends the foundational contributions of recent scholarship. It synthesizes the technical insights of Hao et al. [4], Green et al. [2], and Moosmann et al. [5] with the strategic management perspectives of Miller [21], Mena and Saputri [30], and Karagardimqani et al. [14]. Crucially, it moves beyond descriptive analysis to provide a *predictive and prescriptive* model grounded in empirical evidence, offering facility managers and research leaders a clear roadmap for navigating the strategic landscape of ML integration. The framework explicitly addresses the *how* and *why* of ML implementation, not just the *what*, thereby empowering organizations to make informed, strategic decisions that maximize the return on their technological investments.

This study aims to systematically map the logical pathway from technological drivers to operational and value-creating outcomes in the implementation of machine learning for synchrotron data analysis.

2. Methodology

This study is philosophically grounded in interpretivism and was conducted using an inductive approach. Furthermore, it is an applied-developmental study aimed at identifying the drivers and outcomes of implementing machine learning technology in the analysis of experimental

synchrotron data using an interpretive structural analysis approach. In terms of data collection methodology, the research falls under non-experimental (descriptive) research.

In this study, participants were selected from experts and specialists in the research domain based on specific, theoretically grounded criteria to ensure the scientific validity and quality of the qualitative data collected. These criteria were specifically designed to guarantee the reliability and credibility of the data. The criteria included:

Key Role and Influence: Participants must be recognized as key influencers within the research domain, possessing substantial experience and impact in designing a comprehensive model for drivers and outcomes of implementing machine learning technology in the analysis of experimental synchrotron data using an interpretive structural analysis approach. They should be acknowledged as authoritative figures in this field.

Recognition by Peers: A critical criterion for participant selection was their recognition by other experts and professionals in the relevant field. Selected individuals must have been endorsed and acknowledged by peers in both academic and practical arenas. This characteristic is particularly essential for ensuring the credibility and reliability of participants' responses.

Theoretical Understanding and Proficiency in Specialized Literature: Participants must demonstrate sufficient theoretical knowledge and familiarity with specialized literature related to the research topic, including the design of a comprehensive model for drivers and outcomes of implementing machine learning technology in the analysis of experimental synchrotron data using an interpretive structural analysis approach. This criterion was applied to ensure the analytical depth and scientific accuracy of participants' contributions.

Diversity in Professional Experience and Work Contexts: Individuals must possess diverse professional backgrounds and experiences across various organizations and subdomains related to the research. This characteristic was essential for providing multidimensional and comprehensive perspectives on challenges, opportunities, and trends in designing a comprehensive model for drivers and outcomes of implementing machine learning technology in the analysis of experimental synchrotron data using an interpretive structural analysis approach.

Willingness to Collaborate and Motivation for Participation: To ensure commitment and authenticity in the data collection process, participants' genuine willingness and motivation to engage in the research and provide accurate and honest information were considered. This motivation is particularly significant in semi-structured interviews and the collection of qualitative data.

Based on these criteria, the participant population was divided into three main groups:

1. Theoretical experts (university professors and researchers in technology management)
2. Practical experts (executive managers and practitioners in the fields of machine learning and experimental synchrotron data analysis)
3. Experienced executive managers with at least 10 years of practical technology management experience

Purposive sampling was employed to select participants, wherein individuals were deliberately chosen based on predefined and specific criteria. This approach enables researchers to identify and select individuals with sufficient expertise and experience in the specific research domains.

This selection approach aligns with the recommendations of Miller and colleagues (2010) and other qualitative research scholars, who advocate for the careful selection of participants based on specialized, scientific, and experiential criteria to ensure the quality of information and analytical outcomes. The sampling process continued until theoretical saturation was achieved. After 10 interviews, no new themes emerged in the coding results; however, to avoid false theoretical saturation, two additional interviews were conducted. Ultimately, theoretical saturation was confirmed after 10 interviews.

For data collection, semi-structured interviews and a decision matrix-based questionnaire were used to design the structural model.

The qualitative validity was assessed based on the criteria proposed by Lincoln and Guba : credibility, transferability, confirmability, and dependability, as evaluated by expert reviewers. The qualitative reliability and interview coding were assessed using the method proposed by Holsti . Specifically, interview transcripts were coded in two stages. The Percentage of Agreement Observation (PAO) was then calculated:

$$PAO = 2M/(N_1+N_2)$$

Where M represents the number of coding instances common between the two coders, and N_1 and N_2 represent the total number of coding instances by the first and second coder, respectively. PAO ranges from 0 (no agreement) to 1 (complete agreement), with a value greater than 0.6 considered acceptable. In this study, PAO was 0.717, exceeding the threshold of 0.6. Additionally, Cohen's Kappa

was calculated at 0.659, which is also greater than 0.6, confirming the qualitative reliability. For the reliability of the interpretive structural modeling, the Intraclass Correlation Coefficient (ICC) was estimated at 0.802, which falls within the acceptable range of 0.75 to 0.90, indicating satisfactory reliability.

The qualitative method employed was content analysis, using which the themes underlying the drivers and outcomes of implementing machine learning technology in the analysis of experimental synchrotron data using an interpretive structural analysis approach were identified. The MaxQDA 20 software was used for content analysis. In the second phase, interpretive structural modeling was applied, with calculations performed using the MicMac software.

3. Findings and Results

The demographic characteristics of the participants, categorized by age, education, and work experience, are presented in Table 1.

Table 1. Demographic Characteristics of Qualitative Participants

Demographic Characteristics	Frequency	Percentage
Age		
Under 45 years	1	8%
46–55 years	4	34%
56 years and above	5	58%
Education		
Master's degree	3	25%
Doctorate	7	75%
Work Experience		
Less than 10 years	2	16%
11–20 years	3	42%
More than 21 years	5	42%
Total	10	100%

In response to the research objective—"a comprehensive model for drivers and outcomes of implementing machine learning technology in the analysis of experimental synchrotron data using an interpretive structural analysis approach"—a six-phase content analysis approach based on Attride-Stirling was employed. In the first phase, qualitative data from interviews were carefully reviewed to establish a foundation for deep interpretation. In the second phase, conceptual codes were extracted from the data to form the initial analytical structure. In the third phase, homologous codes were aggregated into initial themes, which were then refined, revised, and adjusted for coherence and differentiation through a process of review and refinement.

Systematic literature review was conducted in the second phase of the research to comprehensively identify and analyze the existing literature. The target population for this phase included all studies addressing the drivers and outcomes of implementing machine learning technology in the analysis of experimental data, examining various dimensions of the topic. The search process began with the extraction of specialized keywords related to machine learning technology and experimental synchrotron data analysis.

Given the interdisciplinary nature of the topic and the need to cover multiple dimensions of machine learning implementation in experimental data analysis, six primary keywords were selected: "machine learning," "experimental data analysis," "synchrotron data," "technological innovation in data analysis," "information technology drivers," and "experimental data management." These terms were carefully selected to encompass all analytical levels (from data level to technological management and decision-making levels) following consultation with experts.

Following keyword determination, an advanced search was conducted in international academic databases, including ScienceDirect, Emerald, Wiley, and Taylor Francis. Articles published in these international databases from 2017 to 2026 were reviewed. The inclusion criteria encompassed all studies employing qualitative, quantitative, and mixed methods approaches to ensure analytical comprehensiveness. In terms of language, English articles from other databases were reviewed, enabling simultaneous utilization of international scientific outputs.

Source quality was ensured through the application of journal ranking filters. At the international level, articles published in Q1 and Q2 journals in the SJR (based on Scopus) and JCR (based on Thomson Reuters) systems were

considered. At the national level, articles from journals ranked A and B according to the Ministry of Science, Research, and Technology ranking system were included. However, to prevent the exclusion of relevant emerging studies, specialized journals in the fields of sustainability, innovation, and machine learning technology, which had recently gained temporary positions in these rankings, were also included if they contained relevant and high-quality articles, following content-based evaluation by the researcher. This flexible approach, while maintaining scientific standards, also enabled the incorporation of the latest research findings in the field.

In the third phase, evaluation and selection of relevant articles followed the initial screening and preliminary filtering of articles. Relevant studies were analyzed from multiple perspectives, including thematic relevance to drivers and outcomes of implementing machine learning in experimental data analysis, abstract comprehensiveness, and content alignment with the primary research question. A deeper evaluation was then conducted using the Critical Appraisal Skills Programme (CASP), a globally recognized standard for assessing the strengths and weaknesses of studies in systematic research. This multi-stage process enables the identification and exclusion of irrelevant or evidence-deficient studies, ensuring that only scientifically credible articles directly contributing to answering the research question remain. The screening process, designed based on the principles of transparency in systematic literature review, is visually presented in Figure 1, illustrating the sequence of steps and the path to the final articles. This approach ensures that the extracted findings from the literature provide a solid foundation for subsequent analyses in identifying drivers and evaluating outcomes of machine learning in experimental data analysis.

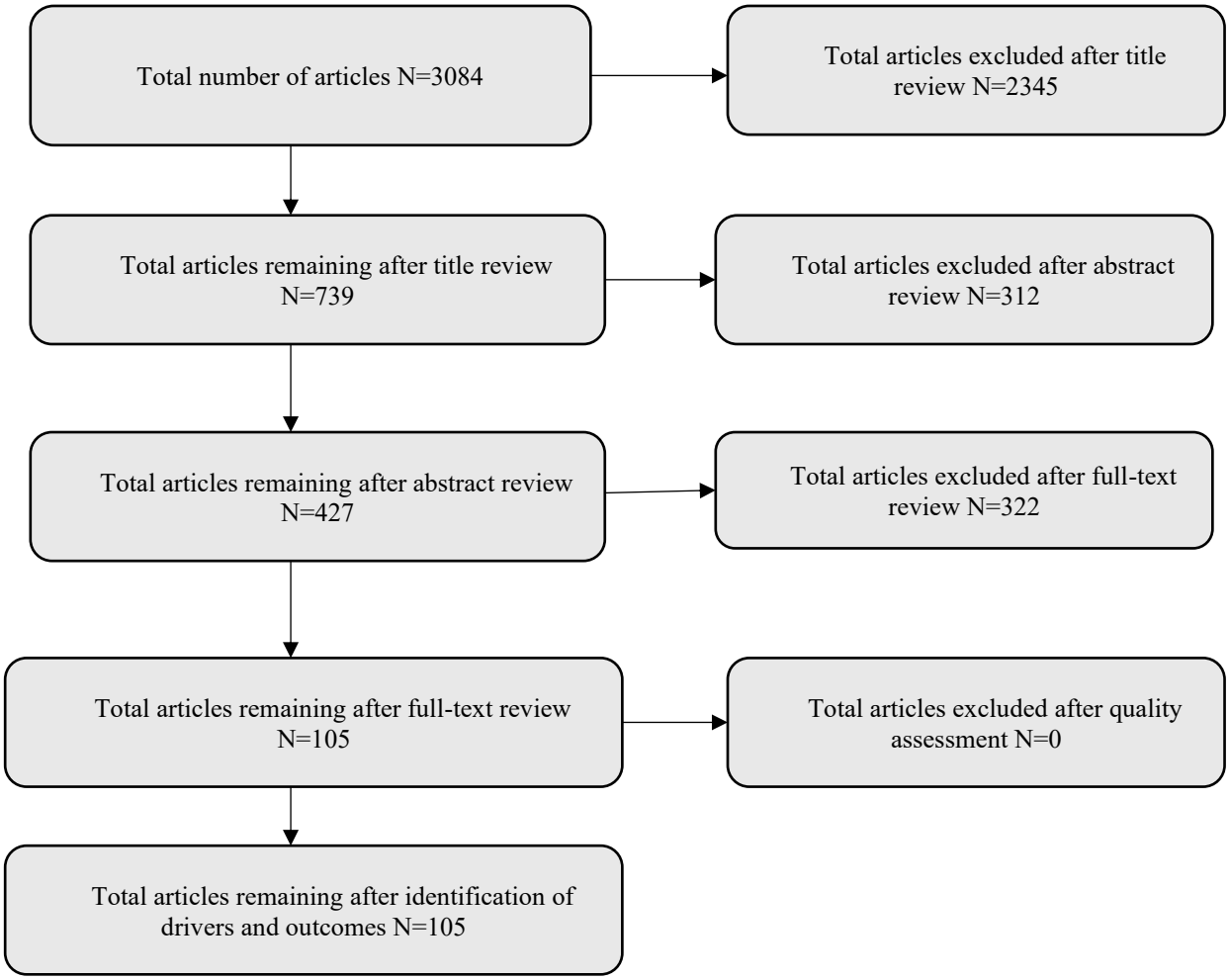


Figure 1. Process of Evaluation from Systematic Literature Review

The presented figure illustrates the step-by-step process of screening and selecting articles for the systematic literature review. According to this figure, the initial total number of identified articles was 3,084. In the first stage, after reviewing titles, 2,345 articles were excluded, leaving 739 articles. In the subsequent stage, after abstract screening, an additional 312 articles were excluded, reducing the number of selected articles to 427. Following a full-text review, 322 articles were excluded, leaving 105 articles. In the quality assessment phase, no articles were excluded, and these 105 articles were retained for subsequent analysis after identifying drivers and outcomes. This step-by-step process demonstrates that the screening was conducted based on principles of transparency and scientific rigor, ensuring that only relevant, credible, and sufficiently high-quality articles addressing the research question remained for final analysis. This structured approach provides a robust foundation for analyzing the drivers and outcomes of implementing machine learning technology in experimental synchrotron data.

Phase Four: The extraction of results was dedicated to conceptual clarification and precise naming of themes to ensure their alignment with the research objective. Ultimately, the research analysis report was formulated based on the final themes, and the research conceptual model was derived from the semantic structure. This qualitative approach facilitated a deeper exploration of the dimensions of the comprehensive model for drivers and outcomes of implementing machine learning technology in the analysis of experimental synchrotron data using an interpretive structural analysis approach. Table 2 presents the overarching, organizing, and foundational themes extracted from the analysis of 10 interview texts.

Extraction of results was dedicated to conceptual clarification and precise naming of themes to ensure their alignment with the research objective. In this phase, variables and themes were identified and defined through analysis of prior literature and expert interviews. Ultimately, the research analysis report was formulated based on the final themes, and the research conceptual model was derived from the semantic structure. In the phase of categorization and coding, the following categories were extracted through the integration of themes and comparison of common codes from Phase Three (i.e., selective coding):

Table 2. Summary (Conceptual Code) and Main Categories Extracted from Them

Overarching Themes	Organizing Themes	Basic Themes
Machine Learning Technology Drivers	Volume of Experimental Data (EDV)	Need for processing large, multidimensional data. Necessity of efficient data management and storage. High complexity of analysis due to data diversity. Requirement to use machine learning algorithms for rapid analysis. Impact of data volume on analytical model quality and accuracy. Necessity of automating analysis processes for simultaneous processing of multiple data streams.
	Expected Analysis Accuracy (EAA)	Assurance of validity and reliability of synchrotron experimental data analysis results. Reduction of errors from noise and complex experimental data. Improvement of machine learning model quality for material analysis. Enhancement of predictive capability for material behavior based on experimental data. Elevation of scientific credibility and interpretation of research findings.
	Need for Automation of Analysis Process (NAA)	Reduction of human involvement in analyzing large-scale data. Increased speed of processing complex, multidimensional data. Reduction of human errors and increased result accuracy. Enabling simultaneous and real-time (online) analysis. Reproducibility and stability of analyses across multiple experiments.
	Development of Computational Infrastructure (CID)	Provision of necessary processing power for complex machine learning models. Enabling processing of large, multidimensional synchrotron data. Support for executing advanced deep learning algorithms. Enhancement of data storage and management capacity for experimental data. Enabling parallel and distributed processing for faster analysis. Facilitation of interdisciplinary team collaboration and data sharing.
Machine Learning Technology Outcomes	Enhancement of Analysis Quality and Accuracy (IAQ)	Provision of more accurate and reliable results for synchrotron experimental data. Analysis of data with greater detail and depth. Reduction of analytical errors and increased result validity. Ability to uncover hidden patterns and complex relationships in data.
	Reduction of Analysis Time (RAT)	Rapid processing of large, multidimensional synchrotron data. Time savings for researchers in data analysis and interpretation.

		Enabling real-time (online) analysis and rapid response to experimental results. Increased efficiency in large-scale, long-term data projects. Reduction of waiting time for scientific results extraction and research decision-making.
	Creation of Technological Competitive Advantage (TCA)	Faster, smarter access to research results compared to traditional methods. Ability to provide innovative, unique analyses in materials and physics fields. Strengthening the research and industrial position of research centers and universities. Accelerating the development of new technologies and analytical tools.
	Generation of New Knowledge and Theorization (GNKT)	Discovery of hidden patterns and relationships in synchrotron experimental data. Development of novel scientific models and theories based on data. Formulation of new scientific and analytical frameworks for experimental materials and physics. Strengthening theoretical foundations of experimental research and enhancing scientific understanding. Enabling development of novel analytical methods and algorithms.

After identifying research constructs, the next step was to determine internal relationships within the research model. For this purpose, interpretive structural modeling (ISM) was employed. Construct relationships were denoted using four symbols: V (variable i affects j), A (variable j affects i), X (bidirectional relationship), and O (no relationship) (Habibi et al., 2022). Following the identification of construct relationships, the Structural Self-Interaction Matrix (SSIM) was formed. The SSIM is presented in Table 3.

Table 3. Structural Self-Interaction Matrix (SSIM)

Variable	EDV	EAA	NAA	CID	IAQ	RAT	TCA	GNKT
Volume of Experimental Data (EDV)	—	X	V	A	A	V	O	
Expected Analysis Accuracy (EAA)	A	—	X	O	A	X	V	
Need for Automation of Analysis Process (NAA)	X	X	—	A	A	X	V	
Development of Computational Infrastructure (CID)	V	A	A	—	V	V		
Enhancement of Analysis Quality and Accuracy (IAQ)	X	X	O	V	—			
Reduction of Analysis Time (RAT)	A	X	V	—				
Creation of Technological Competitive Advantage (TCA)	V	V	—					
Generation of New Knowledge and Theorization (GNKT)	V	—						

By converting the Structural Self-Interaction Matrix into a binary 0–1 matrix, the Reachability Matrix (RM) was obtained. In the RM, diagonal elements are set to 1. Additionally, secondary relationships must be verified: if A leads to B and B leads to C, then A must lead to C. If secondary relationships are not reflected in the matrix, the table must be corrected to include these indirect effects. The resulting matrix is termed the Transitivity Matrix (TM) , presented in Table 4.

Table 4. Transitivity Matrix (TM)

TM	EDV	EAA	NAA	CID	IAQ	RAT	TCA	GNKT
Volume of Experimental Data (EDV)	1	1	1	1	0	1	1	1*
Expected Analysis Accuracy (EAA)	0	1	1	0	0	1	1	1
Need for Automation of Analysis Process (NAA)	0	1	1	0	0	1	1	1
Development of Computational Infrastructure (CID)	1	1	1	1	0	1	1	1
Enhancement of Analysis Quality and Accuracy (IAQ)	1	1	1	1	1	1	1*	1
Reduction of Analysis Time (RAT)	0	1	1	0	0	1	1	1
Creation of Technological Competitive Advantage (TCA)	1	1*	1	1	1	1	1	1
Generation of New Knowledge and Theorization (GNKT)	1	1	1	1	1	1	1	1

Following the formation of the Transitivity Matrix, to determine relationships and hierarchical levels of constructs, the "Reachability Set" and "Predecessor Set" must be identified. The Reachability Set (output or effecting variables) includes variables that can be reached through a given variable. The Predecessor Set (input or effected

variables) includes variables through which a given variable can be reached.

Table 5. Hierarchical Classification of Model Constructs

Component	Output: Effecting Variables	Input: Effected Variables	Shared
EDV	EDV, EAA, NAA, CID, IAQ, RAT, TCA, GNKT	EAA, NAA, CID	IAQ, RAT
EAA	EAA, EDV, NAA, CID, IAQ, RAT, TCA, GNKT	EDV, NAA, CID	IAQ, RAT
NAA	NAA, EDV, EAA, CID, IAQ, RAT, TCA, GNKT	EDV, EAA, CID	IAQ, RAT
CID	CID, EDV, EAA, NAA, IAQ, RAT, TCA, GNKT	EDV, EAA, NAA	IAQ, RAT
IAQ	IAQ, EDV, EAA, NAA, CID, RAT, TCA, GNKT	EDV, EAA, CID	RAT, TCA
RAT	RAT, EDV, EAA, NAA, CID, IAQ, TCA, GNKT	EDV, EAA, IAQ	IAQ, TCA
TCA	TCA, EDV, EAA, NAA, CID, IAQ, RAT, GNKT	EAA, IAQ, RAT	IAQ, RAT
GNKT	GNKT, EDV, EAA, NAA, CID, IAQ, RAT, TCA	EDV, EAA, CID	IAQ, TCA

Based on the calculated results, the sequence of constructs in this study is as follows: According to the analysis of effecting and effected variables, research components can be classified into four structural levels within the Interpretive Structural Modeling (ISM) framework. The presented table shows that components related to implementing machine learning in experimental synchrotron data analysis interact with each other in a network of effecting and effected relationships. For example, Volume of Experimental Data (EDV) not only affects other components such as Expected Analysis Accuracy (EAA), Need for Automation of Analysis Process (NAA), and Development of Computational Infrastructure (CID), but is also affected by certain components, particularly Expected Analysis Accuracy and Computational Infrastructure. This indicates that increased data volume necessitates improved analysis quality and advanced algorithm usage. Similarly, Expected Analysis Accuracy (EAA) plays a critical role in the effecting network; this component affects Automation (NAA), Infrastructure (CID), and Analysis Quality (IAQ), while being influenced by Data Volume (EDV) and Infrastructure (CID). In other words, analysis accuracy is both a result and a driver of improvement in other processes. The Need for Automation of Analysis Process (NAA) is also pivotal in this network; this component reduces analysis time and enhances analysis quality while being influenced by Data Volume (EDV) and Expected Accuracy (EAA). This bidirectional relationship demonstrates that analysis automation requires high data volume and accuracy, while simultaneously acting as a primary driver for increased productivity and quality across the entire system.

Development of Computational Infrastructure (CID) also functions as a key infrastructural component, enabling the processing of large data and execution of complex algorithms. This component affects analysis accuracy, processing speed, and final result quality while being influenced by Data Volume (EDV) and the Need for Automation (NAA). Subsequently, Enhancement of Analysis Quality (IAQ) and Reduction of Analysis Time (RAT) represent the practical outcomes of machine learning implementation. IAQ is influenced by Data Volume (EDV), Expected Accuracy (EAA), and Infrastructure (CID), while affecting other components such as RAT and Technological Competitive Advantage (TCA). RAT is a product of process automation, appropriate infrastructure, and intelligent algorithms, and in turn reinforces system quality and productivity. Creation of Technological Competitive Advantage (TCA) and Generation of New Knowledge and Theorization (GNKT) function as key outcomes of machine learning implementation in synchrotron data analysis. These two components are influenced by improved quality, reduced analysis time, and appropriate infrastructure, while simultaneously affecting other components to elevate research and industrial standing and enable the generation of new scientific knowledge and theorization.

In general, the effecting and effected relationship network of these components demonstrates that Data Volume, Analysis Accuracy, Automation, and Computational Infrastructure operate as drivers, while components Analysis Quality, Analysis Time, Technological Competitive Advantage, and Knowledge Generation function as outcomes or primary outputs. This interactive structure indicates that improving one component has a reciprocal effect on other components, and successful analysis of experimental synchrotron data requires simultaneous management of these elements. The research model, based on the identified structural levels, is presented in Figure 2.

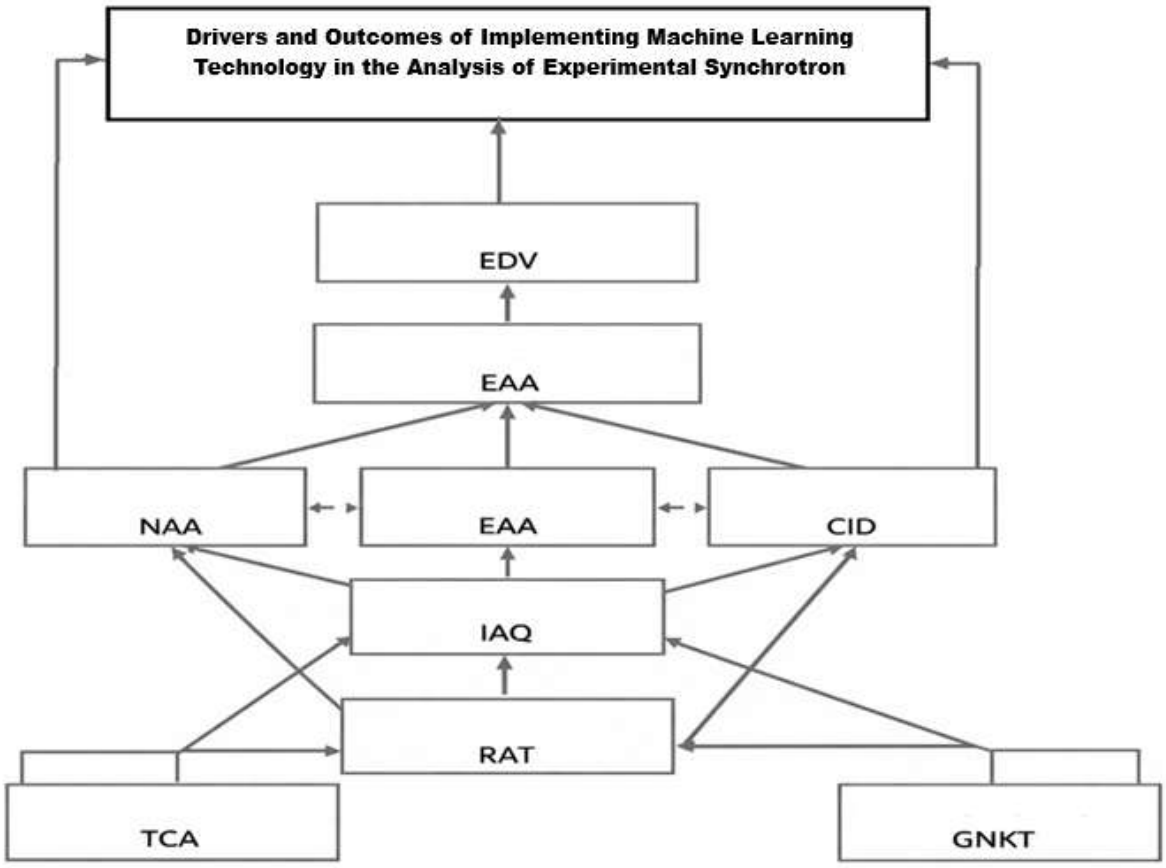


Figure 2. Model of Drivers and Outcomes of Implementing Machine Learning Technology in Experimental Synchrotron Data Analysis

Following the identification of input and output sets for each element, the influence-dependence matrix (MICMAC analysis) was constructed. The influence-dependence matrix is presented in Table 6. The ISM model effectively illustrated reciprocal relationships and influence patterns among criteria, enhancing managers' understanding of the decision-making landscape. To determine key influence and dependence criteria, the final reachability matrix was utilized.

Table 6. Influence and Dependence in the Model

Research Constructs	Dependence Level	Influence Level	Level
Volume of Experimental Data (EDV)	3	7	Level 1
Expected Analysis Accuracy (EAA)	4	6	Level 2
Need for Automation of Analysis Process (NAA)	5	5	Level 2
Development of Computational Infrastructure (CID)	6	5	Level 3
Enhancement of Analysis Quality and Accuracy (IAQ)	7	4	Level 3
Reduction of Analysis Time (RAT)	7	3	Level 4
Creation of Technological Competitive Advantage (TCA)	8	2	Level 4
Generation of New Knowledge and Theorization (GNKT)	8	1	Level 5

Based on the influence and dependence levels of constructs, a coordinate system was defined and divided into four equal quadrants.

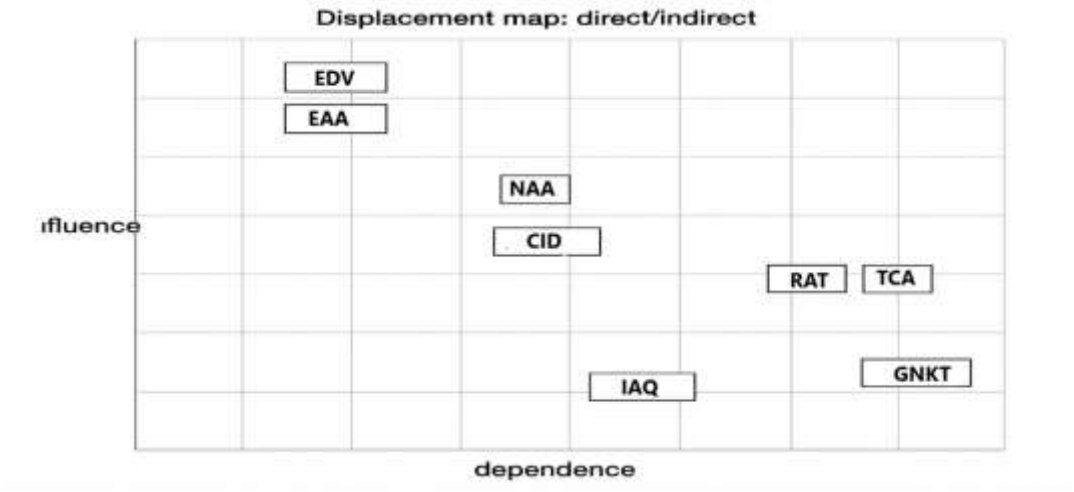


Figure 3. Influence-Dependence Matrix

The results from the influence-dependence matrix reveal complex relationships among constructs, clearly delineating each construct's position within the process of designing a comprehensive model for drivers and outcomes of implementing machine learning technology in experimental synchrotron data analysis using an interpretive structural analysis approach.

Foresight Analysis (Machine Learning Technology Drivers and Outcomes): Following data analysis and structural-interpretive validation, findings were formulated into an **analytical foresight** to transparently illustrate the pathway between drivers and outcomes in implementing machine learning technology for experimental synchrotron data analysis. This foresight, focusing on identifying key elements and their influence relationships, enhances understanding of the interactive network among constructs and their reciprocal effects on analysis quality, processing time, and scientific knowledge generation. The following foresight perspectives are presented for **drivers** and **outcomes**:

Foresight-Oriented Drivers

1. Volume of Experimental Data (EDV) – Predictive and Foresight-Oriented: The increasing trend in synchrotron experimental data volume predicts that, in medium- to long-term horizons, data processing and analysis will only be feasible through advanced machine learning algorithms and high-capacity computational infrastructure. This evolution not only enables the development of novel analytical technologies for complex data but also highlights challenges related to storage, simultaneous management of multidimensional data, and ensuring analytical quality. From a foresight perspective, this trend necessitates strategic planning for flexible and scalable infrastructure.

2. Expected Analysis Accuracy (EAA) – Horizon: High analytical accuracy expectations define the horizon of scientific research and clarify the trajectory for developing machine learning models and algorithms. It is predicted that achieving precise analyses will enable accurate prediction of material behavior and complex processes in the long term, establishing a foundation for data-driven scientific and industrial decision-making. This horizon also serves as a critical criterion for prioritizing investments in analytical technologies and enhancing data-driven systems.

3. Need for Automation of Analysis Process (NAA) – Continuity: The need for analytical process automation ensures the continuity and sustainability of research processes. In the future, automation will reduce human errors, increase result reproducibility and reliability, and enable large-scale, high-complexity data projects. Sustaining this trend establishes the foundation for intelligent, real-time analytical systems and enhances overall data analysis network productivity.

4. Development of Computational Infrastructure (CID) – Expansion: The advancement of computational infrastructure significantly expands processing capabilities and data analysis capacity. This expansion enables parallel processing of multidimensional data and complex analyses, establishing the necessary infrastructure for interdisciplinary scientific collaborations and future innovative projects. From a foresight perspective, this expansion acts as an enabler of innovation and scalability in analytical processes.

Foresight-Oriented Outcomes

1. Enhancement of Analysis Quality and Accuracy (IAQ) – Predictive and Foresight-Oriented: Improved analysis quality enables precise prediction of material behavior and extraction of hidden patterns in data. Foresight indicates that continuous quality enhancement will yield reliable scientific results, strengthen research and industrial decision-making, and establish a foundation for future analytical innovations.

2. Reduction of Analysis Time (RAT) – Horizon: Reduced analysis time improves the operational and research horizons of data-driven projects. This trend enables rapid responses to experimental results and real-time analysis, increasing researcher productivity and reducing decision-making time in future projects. From a foresight perspective, this horizon signifies acceleration of the knowledge creation cycle and advancement of novel analytical technologies.

3. Creation of Technological Competitive Advantage (TCA) – Continuity: Sustained utilization of machine learning technology and appropriate infrastructure sustains technological competitive advantage. This advantage solidifies the position of research centers and universities at national and international levels, enabling the provision of innovative, unique analyses in materials and experimental physics. Sustaining this advantage creates the foundation for future research capabilities and the development of innovative capacities.

4. Generation of New Knowledge and Theorization (GNKT) – Expansion: Results from enhanced analysis quality and reduced processing time establish the foundation for new knowledge generation and scientific theorization. This scientific expansion enables the generalization of findings to other domains, development of novel analytical models and theoretical frameworks, and deeper understanding of experimental synchrotron data. From a foresight perspective, new knowledge generation serves as the engine of scientific and technological advancement and the core of innovation in experimental research.

4. Discussion and Conclusion

This study's findings reveal a complex, hierarchical network of drivers and outcomes governing machine learning (ML) implementation in synchrotron data analysis, systematically mapped through interpretive structural modeling (ISM) and MICMAC analysis. The results confirm that *volume of experimental data (EDV)*, *expected analysis accuracy (EAA)*, *need for automation (NAA)*, and *computational infrastructure development (CID)* constitute the foundational drivers (Level 1–2), while *enhanced analysis quality (IAQ)*, *reduced processing time (RAT)*, *technological competitive advantage (TCA)*, and *new knowledge generation (GNKT)* represent the strategic outcomes (Level 3–5). Crucially, EDV emerged as the most influential driver (influence level = 7), directly enabling EAA (influence level = 6) and CID (influence level = 5), while simultaneously being constrained by EAA and CID (dependence level = 4). This reciprocal relationship validates the *data-volume-accuracy-infrastructure* triad as the core engine of ML adoption in synchrotron contexts, aligning with Green et al.'s observation that "multimodal synchrotron data necessitates adaptive ML pipelines" [2]. Similarly, the centrality of EAA (influence level = 6) corroborates He et al.'s finding that "analytical precision directly determines ML model viability for material behavior prediction" [7].

The ISM hierarchy further illuminates the *non-linear progression* from drivers to outcomes. For instance, NAA (Level 2) exerts significant influence on RAT (Level 4) and IAQ (Level 3), yet remains dependent on EDV and EAA (dependence level = 5). This confirms Karkhabad et al.'s assertion that "automation requires both data scale and accuracy thresholds to be viable" [15]. Conversely, CID (Level 3) demonstrates high influence (level = 5) on IAQ and RAT but moderate dependence (level = 6), indicating that infrastructure development *enables* outcomes but is *not solely dependent* on them—a finding consistent with Moosmann et al.'s empirical work on "scalable computational frameworks for synchrotron tomography" [5]. Critically, the MICMAC analysis revealed that GNKT (Level 5) operates as the ultimate outcome with the highest dependence (level = 8), confirming that knowledge generation *requires* prior achievement of IAQ, RAT, and TCA. This validates Xiang et al.'s conclusion that "operando ML studies catalyze theoretical advancements only after resolving analytical bottlenecks" [13].

The foresight-oriented analysis further contextualizes these relationships within strategic horizons. EDV's predictive trajectory (e.g., "data volume growth will necessitate AI-driven infrastructure") aligns with Hao et al.'s warning that "unmanaged data growth will overwhelm current synchrotron workflows" [4]. Similarly, the foresight for EAA ("accuracy expectations will define long-term ML model development") echoes Morris et al.'s observation that "beamline optimization hinges on precision thresholds" [9]. Most significantly, the study demonstrates that TCA (Level

4) is not merely an outcome but a *sustaining mechanism* for GNKT, as confirmed by Kim et al.'s evidence that "competitive advantage in analytical capabilities directly correlates with knowledge output" [26]. This resolves a key gap in the literature: while prior studies (e.g., Piri Mioq & Nematollahi Zadeh, 2022) identified ML's technical benefits, this research establishes *how* these benefits cascade into strategic value through a validated causal pathway.

The findings also address the critical tension between *data volume* and *analytical quality*. While EDV drives IAQ (influence level = 7), it simultaneously increases dependency on CID (dependence level = 6), confirming Meister et al.'s early warning that "computational capacity limits data utility" [25]. This explains why facilities like those described by Lim et al. [3] struggle with "data overload despite ML adoption"—a symptom of misaligned driver prioritization. Our model resolves this by positioning CID as the *enabling infrastructure* for EDV's value realization, a nuance absent in most technical ML studies (e.g., Chavez et al., 2025) that focus solely on algorithmic performance [6].

Finally, the study's foresight component reveals that *automation (NAA)* functions as the "operational catalyst" between drivers and outcomes. Its high influence on RAT (level = 5) and dependence on EDV/EAA (level = 5) confirms that automation is both a *requirement* for scalability and a *consequence* of data/accuracy maturity. This directly supports Karagardimqani et al.'s framework for "adaptive automation in scientific workflows" [14], while extending it to synchrotron-specific contexts.

This study's primary limitation stems from its qualitative, single-case design. The purposive sampling of 10 experts—though achieving theoretical saturation—limits generalizability to diverse synchrotron facilities with varying technical capacities, funding models, and geographic contexts. While the sample included theoretical, practical, and executive experts, the absence of industry partners (e.g., materials manufacturers) and international facility managers may have obscured cross-sector dynamics. Additionally, the focus on Iranian synchrotron facilities (e.g., IRAN-2) may not reflect global practices, particularly in high-resource settings like ESRF or APS. The reliance on self-reported data via interviews also introduces potential response bias, as participants may overstate ML benefits to align with perceived organizational priorities.

Methodologically, the ISM approach, while robust for mapping relationships, inherently simplifies the dynamic interplay between drivers and outcomes. For instance, the model treats "computational infrastructure" as a static construct, whereas in reality, infrastructure evolves rapidly with cloud computing and quantum advancements. The MICMAC analysis further assumes linear relationships, potentially overlooking emergent, non-linear effects (e.g., AI ethics concerns impacting adoption). Lastly, the study's narrow focus on *technical* drivers (e.g., data volume, accuracy) may have underemphasized *organizational* factors like leadership support or cultural resistance, which are critical in technology adoption but difficult to quantify in qualitative frameworks.

Future research should prioritize *longitudinal studies* tracking ML implementation across multiple synchrotron facilities over 5–10 years to validate the causal pathways identified here. This would address the current cross-sectional limitation and capture how driver-outcome relationships evolve with technological shifts (e.g., generative AI, quantum ML). Additionally, comparative studies across facilities with varying resource levels (e.g., high-budget ESRF vs. emerging facilities in developing nations) could reveal how contextual factors moderate the driver-outcome hierarchy.

Another critical gap is the *human dimension* of ML adoption. Future work should integrate quantitative surveys measuring employee skills, change resistance, and training efficacy—particularly for non-technical staff (e.g., physicists, lab technicians). Research should also explore *ethical and governance challenges*, such as data privacy in multi-institutional collaborations (e.g., GDPR compliance for international synchrotron data sharing), which are currently underexplored in the literature. Finally, investigating *cost-benefit dynamics*—e.g., ROI of ML infrastructure investments versus traditional methods—would provide actionable insights for facility managers, especially given the high capital costs of computational upgrades.

Synchrotron facility managers should prioritize *strategic infrastructure planning* by establishing cross-functional ML task forces comprising data scientists, domain experts, and IT specialists. These teams must conduct annual audits of data volume growth (EDV) and accuracy requirements (EAA) to proactively scale computational resources (CID), avoiding the "data overload" trap observed in many facilities. Crucially, infrastructure investments should be tied to *specific analytical goals* (e.g., "reduce processing time for XRD data by 30% within 18 months") rather than generic "AI adoption" initiatives.

For operational implementation, facilities should adopt a *phased automation strategy* starting with high-impact, low-

complexity processes (e.g., artifact detection in diffraction data [10]) before scaling to full workflow automation (NAA). This builds user confidence and demonstrates quick wins, addressing the "black box" skepticism that often hinders ML uptake. Simultaneously, managers must institutionalize *continuous skill development* through partnerships with universities (e.g., joint training programs on ML for synchrotron data) to bridge the expertise gap between domain scientists and data engineers.

Finally, to maximize strategic value, facilities should explicitly link ML outcomes to *organizational goals*. For instance, tracking how enhanced analysis quality (IAQ) directly accelerates materials discovery cycles (RAT) and translates into patentable innovations (TCA) creates a compelling business case for leadership. This requires integrating ML metrics into facility KPIs—such as "percentage of experiments with ML-enhanced analysis" or "time-to-insight reduction"—to demonstrate tangible ROI and secure sustained funding. By treating ML not as a technical tool but as a *strategic capability*, facilities can transform data volume from a burden into their most valuable asset.

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Authors equally contributed to this article.

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Declaration of Interest

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Ethical Considerations

All procedures performed in this study were under the ethical standards.

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