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Analysis of Perception and Knowledge on Chemometric Competence among Students and Practitioners Using SEM–PLS

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ABSTRACT

The advancement of digital technology and data driven analysis in the 21st century has fundamentally transformed science education. The growing integration of coding, artificial intelligence (AI), and deep learning requires learners to develop strong computational and analytical thinking skills. Chemometrics has emerged as a key interdisciplinary field that integrates mathematics, statistics, and computer science to support scientific data interpretation, making it an essential competence in modern research and education. This study explores the relationships among perception, knowledge, and chemometric competence among students and practitioners to identify key factors that enhance data analysis skills in AI based learning environments. Data were collected using Google Forms from participants across various academic levels and professional backgrounds and analyzed using the structural equation modeling–partial least squares (SEM–PLS) approach. The findings indicate that positive perceptions and adequate knowledge play a significant role in strengthening chemometric competence. These results underscore the importance of integrating chemometrics into science education curricula to enhance analytical literacy and prepare learners for data-intensive and AI driven scientific challenges.

Keywords: Artificial Intelligence, Chemometrics, Competence, Perception, SEM–PLS.

Introduction

Perceptions and knowledge of chemometrics play an essential role in shaping the scientific competencies of students and practitioners. Perception reflects an individual's views regarding the benefits and relevance of chemometrics in research and data analysis, while knowledge relates to conceptual understanding, technical skills, and the ability to apply chemometric methods (Brereton et al., 2018). Previous studies indicate that strong knowledge and positive perceptions of chemometrics enhance individuals' readiness to apply these methods to effectively interpret complex datasets. Therefore, developing sound conceptual understanding and appropriate perceptions of chemometrics constitutes a critical foundation in modern scientific education.

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Chemometrics, as a multivariate analytical method is closely linked to the development of artificial intelligence (AI) and machine learning. The analysis of large and complex datasets, which characterizes AIdriven research, requires multivariate statistical techniques to extract meaningful information (Joshi, 2023; Kharbach, 2025). The integration of chemometrics with AI not only improves analytical accuracy but also strengthens predictive capabilities and data-driven decision-making. Numerous studies demonstrate this application: Rafi et al. (2021) used PCA and PLS regression to identify functional groups contributing to the antioxidant activity of Sonchus arvensis leaves; Rafi et al. (2022) applied NIR and OPLS-DA to authenticate Cymbopogon nardus essential oil; Rohman et al. (2021) utilized PCA and PLSR for the classification of Sida rhombifolia and prediction of radical scavenging activity; and Rafi et al. (2020) employed NIR and PCA-DA to discriminate cassava, taro, and wheat flour. These examples demonstrate that chemometrics is effective for classification, prediction, and authentication based on spectral data and supports the advancement of modern scientific analytical methods.

The application of chemometrics and SEM–PLS has been utilized in a variety of fields to evaluate competencies, attitudes, and behaviors in both professional and academic contexts. Previous studies show that chemometrics has been used to assess the quality of medicinal plants through combinations of HPLC, GC, NMR, UV, and IR methods, as well as for taxonomic discrimination and geographic-origin classification (Shafirany et al., 2018). SEM–PLS has also been applied to analyze the competencies of traditional fishermen in Banten Bay, where skills were the most influential factor, and knowledge influenced both skills and self-perception (Noviyanti & Nurhasanah, 2019). Furthermore, several studies have used SEM–PLS in educational and professional settings, including: Rahardjo (2022), who analyzed relationships among competency, perception, and interest in the public accounting profession with motivation as a mediator; Tjahjadi (2024), who evaluated the effect of perception on leadership quality and electability in regional elections; Masdoki (2024), who assessed Teacher 4.0 competencies based on the DigCompEdu model; Hendriyani (2025), who showed the influence of lecturer competence on motivation and student achievement; and González-Medina et al. (2025) who emphasized the importance of digital teaching competence for empowering university students. Abreh et al. (2025) further demonstrated that AI literacy and environmental support are critical for STEM students' intention to learn AI. Additionally, Joshi (2023) explained that chemometrics and machine learning are driving transformation in chemistry despite challenges related to data complexity and reproducibility, while Kharbach (2025) highlighted that AI integration enhances the power of classical chemometrics to address large datasets. Applications of chemometrics in chemical science are also reflected in studies such as Rafi et al. (2020, 2021, 2022) and Abdul et al. (2021), who used PCA, PLS, and OPLS-DA for the analysis of phenolic content, antioxidant activity, and authentication of herbal and essential oil products. Moreover, Koteczki and Balassa (2025) showed that the acceptance of AI among university students is influenced by psychological, technological, and social factors, with positive user experience being the strongest predictor, highlighting the importance of user-friendly AI tools and support tailored to student attitudes. Overall, this body of research confirms that SEM–PLS is effective for analyzing relationships among perception, competence, and digital or AI literacy, yet it has not been specifically applied to chemometric competence, despite the field's growing importance in the integration of machine learning and modern scientific data analysis.

Based on this background, the present study aims to analyze the relationships among perception, knowledge, and the application of chemometrics with respect to the data analysis competencies of students and practitioners. The study also explores the mediating role of data analysis competence and the moderating effect of learning facility support in strengthening the influence of independent variables on chemometric competence. It is expected that the findings will provide deeper empirical insights into the factors that foster analytically oriented literacy grounded in chemometrics and AI.

Research Methods

Research Framework

This research adopts a quantitative survey methodology to investigate the relationships among variables within a structural model that underscores the importance of chemometric scientific competence. A quantitative approach was chosen because it facilitates systematic and objective evaluation of causal relationships. The research framework was comprehensively structured by integrating independent, dependent, mediating, moderating, and control variables to provide an in-depth understanding of the factors shaping chemometric competence. Data analysis was conducted using structural equation modeling–partial least squares (SEM–PLS) which is well suited for exploratory studies involving complex models, ideal sample sizes, and relaxed assumptions regarding data normality (Hair et al., 2021). The study population consisted of students across diploma (D4), undergraduate (S1), master's (S2), and doctoral (S3) programs, as well as practitioners working in chemistry related disciplines. A total of 100 potential respondents were identified. Referring to the minimum sample size rule for PLS-SEM proposed by Hair et al. (2021), which recommends at least ten times the maximum number of structural paths directed at a single endogenous construct, the model required a minimum of 80 respondents. Accordingly, the sampling strategy was designed to meet this requirement and ensure sufficient statistical power.

Primary data were collected using an online questionnaire distributed via Google Forms. The questionnaire was developed based on theoretically grounded indicators derived from prior literature. All measurement items employed a seven point Likert scale ranging from 1 (strongly disagree) to 7 (strongly agree) enabling respondents to accurately express their perceptions, knowledge, and application of chemometrics in both academic and professional contexts (Joshi et al., 2015). This study involved nine latent variables. The independent variables included: (1) perception of chemometrics (X1), reflecting respondents views on the role and benefits of chemometrics in scientific research; (2) knowledge of chemometrics (X2), representing conceptual understanding and technical proficiency; and (3) application of chemometrics in data analysis (X3), indicating the extent of practical implementation. The dependent variable was the perceived importance of chemometrics in research (Y), measuring its contribution to research accuracy and efficiency. Data analysis competence (Me) served as a mediating variable, capturing respondents ability to interpret and manage complex data structures, while learning and research facility support (Mo) functioned as a moderating variable, assessing the influence of institutional infrastructure. Additionally, three control variables academic background (K1), research experience (K2), and industrial relevance of chemometrics (K3) were included to account for potential external influences on the primary model (Hair et al., 2021).

Data analysis was performed using SmartPLS version 4 following the two stage SEM–PLS procedure. In the first stage, the measurement model was assessed by examining indicator reliability through outer loading values (≥ 0.70), internal consistency using Cronbach's Alpha and Composite Reliability (≥ 0.70) and convergent validity via the average variance extracted (AVE ≥ 0.50). Discriminant validity was evaluated using the Fornell–Larcker criterion and the Heterotrait–Monotrait (HTMT) ratio, with values below 0.85 indicating acceptable discriminant validity (Hair et al., 2021). Overall, this methodological approach was designed to generate robust empirical evidence regarding the determinants of chemometric competence among students and practitioners, while addressing the existing research gap related to the application of SEM–PLS in chemometrics-oriented competence studies. The subsequent table presents the variables and indicators employed in the SEM–PLS measurement model.

Table 1. Variable and Indicator for SEM-PLS

Type of Variable	**Variable code**	**Variable name**	**Indicator**	**Indicator code**
Independent	X1	Perception of Chemometrics	1. Chemometrics is considered important in chemical research and data analysis	X1.1, X1.2, X1.3

			2. Chemometrics helps improve the efficiency of laboratory analysis 3. Understanding chemometrics enhances the quality of research outcomes	
Independent	X2	Knowledge of Chemometrics	1. I understand the basic concepts and applications of chemometrics 2. I am able to use chemometric software or methods 3. I have participated in training or learning activities related to chemometrics	X2.1, X2.2, X2.3
Independent	X3	Application of Chemometrics in Data Analysis	1. I apply chemometric methods in research or laboratory practice 2. I understand the statistical analysis results from chemometrics 3. I can correctly interpret the results of chemometric models	X3.1, X3.2, X3.3
Dependent (Y)	Y	Importance of Chemometrics in Research	1. Chemometrics plays an important role in scientific decision-making 2. Chemometrics improves the accuracy and reliability of research results 3. Chemometrics facilitates multivariate analysis and data interpretation	Y.1, Y.2, Y.3
Mediator (Me)	Me	Data Analysis Competence	1. I am able to analyze experimental data accurately 2. I have skills in using statistical analysis tools. 3. I understand the relationships between variables in the data	Me.1, Me.2, Me.3
Moderating (Mo)	Mo	Support for Learning and	1.Computer facilities and analysis software are readily available	Mo.1, Mo.2, Mo.3

		Research Facilities	2.The institution provides support for chemometrics learning 3.Access to data and learning resources for chemometrics is easily obtainable	
Control (K1)	K1	Academic Background	1. Formal education level related to chemistry or data analysis 2.Experience in learning analytical chemistry/chemometrics. 3.Frequency of using statistical analysis in studies	K1.1, K1.2, K1.3
Control (K2)	K2	Research Experience	1.The number of research projects conducted 2.Types of research involving complex data analysis 3.Involvement in data-based scientific publications	K2.1, K2.2, K2.3
Control (K3)	K3	Importance of Chemometrics in Industry	1. Chemometrics is used for product quality control 2.Chemometrics helps improve industrial process efficiency 3.Chemometrics supports data-driven innovation in production	K3.1, K3.2, K3.3

Results and Discussion

SEM–PLS Model

The research model developed in this study illustrates the interrelationships among variables forming a conceptual framework for strengthening analytical literacy based on artificial intelligence (AI) through the integration of chemometrics in science education. In general, the model was constructed using the Structural Equation Modeling–Partial Least Squares (SEM–PLS) approach, consisting of independent, dependent, mediating, moderating, and control constructs (Figure 1). Three core constructs function as independent variables (X1, X2, X3) namely perception of chemometrics (X1), knowledge of chemometrics (X2), and chemometric competence (X3). Each construct is measured using three reflective indicators (X1.1–X1.3, X2.1–X2.3, and X3.1–X3.3). These variables represent cognitive aspects and scientific skills required by students and practitioners in applying chemometric methods, coding, and AI-based data analysis in science learning. The relationships among these constructs are assumed to have a direct influence on the dependent variable (Y) namely AI-based scientific data analysis capability, measured through indicators Y.1, Y.2, and Y.3. Between the independent and dependent variables lies a mediating variable (Me) measured through three indicators (Me.1–Me.3). This variable explains the indirect influence of perception and knowledge on scientific analytical capability. In this context, the mediator can be interpreted as AI-based learning motivation or self efficacy in data analysis, which strengthens the linkage between conceptual understanding and the practical application of chemometric techniques. Additionally, a moderating variable (Mo) with three indicators (Mo.1–Mo.3) is included to test whether the relationships between the independent and dependent variables are strengthened or weakened by external factors. This moderator represents digital literacy and technological experience, determining the extent to which perception and knowledge can be translated into actual chemometric competence. Three further variables—K1, K2, and K3—are positioned as control variables to ensure that the relationships among the main constructs are not distorted by external influences. Each contains three indicators (K1.1–K3.3) describing demographic factors, experience using data analysis software, and the intensity of technology utilization in learning or research. Directional paths in the model represent causal relationships among variables, such as the direct effects of X1, X2, and X3 on Y, the indirect effects through the mediator (Me), and interaction effects through the moderator (Mo). The inclusion of control variables increases the model's validity by ensuring that estimation results are not biased due to respondent background differences. Conceptually, the model demonstrates that strengthening chemometric competence depends not only on cognitive components such as perception and knowledge, but also on psychological mechanisms (motivation/mediator) and digital adaptive capacity (moderator). This integrative approach reflects a 21st-century learning paradigm that demands the synergy of analytical skills, computational thinking, and readiness to engage with AI-driven transformation in science education.

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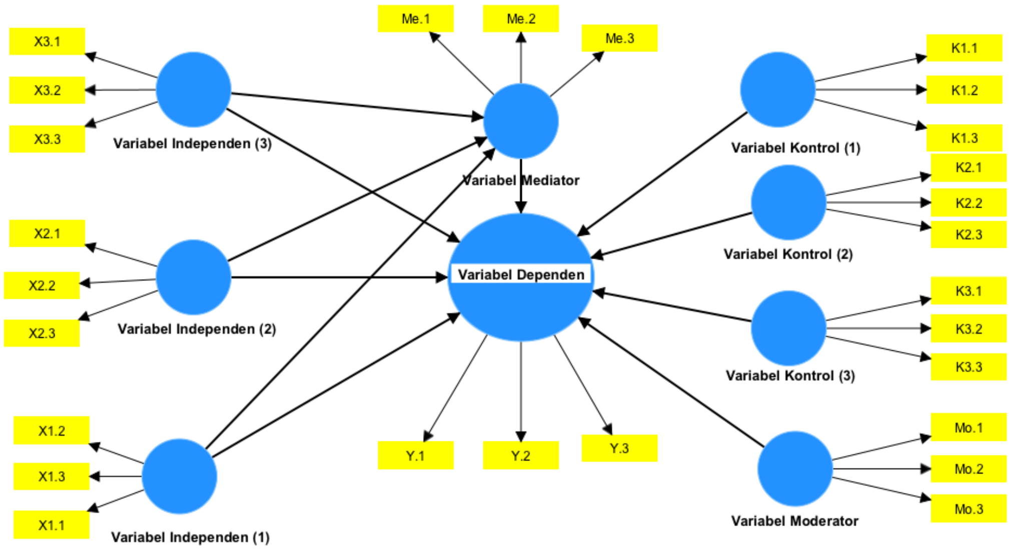

Figure 1. Relationship variable (Blue) and indicator (yellow) in SEM-PLS model

Table 2. SEM-PLS without *bootstraping*

	Loading factor	AVE	rho_a (composite reability)	Cronbach's alpha	rho_c (composite reability)	VIF
Acceptance Criteria	**>0,7**	**>0,5**	**<5**	**>0,7**	**<5**	**<5**
Indicator			**Independent variable 1 (X1)**			
X1.1	0,932	0,818	0,902	0,888	0,931	3,677
X1.2	0,841					1,934
X1.3	0,938					3,839
Indicator			**Independent variable 2 (X2)**			
X2.1	0,937	0,914	0,955	0,953	0,969	4,134
X2.2	0,970					7,878
X2.3	0,960					6,387
Indicator			**Independent variable 3 (X3)**			
X3.1	0,929	0,924	0,963	0,959	0,973	3,674
X3.2	0,978					16,446
X3.3	0,976					15,755
Indicator			**Dependent variable (Y)**			
Y.1	0,906	0,714	0,827	0,790	0,880	3,430
Y.2	0,933					3,712
Y.3	0,670					1,257
Indicator			**Control variable (1)**			
K1.1	0,813	0,713	0,914	0,804	0,881	1,740
K1.2	0,790					1,618
K1.3	0,925					2,043
Indicator			**Control variable (2)**			
K2.1	0,832	0,730	0,873	0,825	0,890	2,324
K2.2	0,865					1,561

K2.3	0,867					2,195
Indicator			**Control variable (3)**			
K3.1	0,919	0.876	0,930	0,929	0,955	3,116
K3.2	0,953					4,889
K3.3	0,935					4,058
Indicator			**Mediator variable**			
Me.1	0,927	0,882	0,937	0,933	0,957	3,711
Me.2	0,953					4,821
Me.3	0,937					3,653
Indicator			**Moderating variable**			
Mo.1	0,918	0,761	0,861	0,842	0,905	2,647
Mo.2	0,895					2,484
Mo.3	0,799					1,620

Results of the Outer Model Evaluation

The evaluation of the outer model was conducted on the reflective constructs X1, X2, X3 (independent), Y (dependent), Mo (moderator), Me (mediator), and K1–K3 (control), using indicators measured on a 7-point Likert scale. Convergent validity was assessed through outer loadings and average variance extracted (AVE), reliability through composite reliability (CR) and Cronbach's alpha, while local multicollinearity was evaluated using the variance inflation factor (VIF). According to Hair et al. (2021), outer model evaluation criteria include convergent validity, discriminant validity, and construct reliability, all of which must be satisfied before structural analysis is performed. The results show that all indicators have dominant outer loadings on their respective constructs, with values above 0.70, except for Y3 (0.670), which remains acceptable. All constructs also met the required thresholds of AVE $\geq$ 0.50 and CR $\geq$ 0.70, indicating adequate convergent validity and construct reliability (Fornell & Larcker, 1981). The AVE values ranged from 0.713 to 0.924, demonstrating that each construct explains more than 50% of the variance of its indicators.

Discriminant validity, assessed using the heterotrait–monotrait ratio (HTMT), showed that all construct pairs were below the recommended cut-off of 0.85/0.90, indicating sufficient discriminant separation. Cross-loading results also confirmed that the highest loading of each indicator was found on its designated construct, further supporting discriminant validity (Fornell & Larcker, 1981). Collinearity testing revealed that most indicators had VIF values < 5. However, in constructs X2 and particularly X3, several indicators exhibited VIF values > 5, indicating redundancy among indicators. High multicollinearity can reduce the clarity of the measurement model. Based on common decision rules (loading < 0.70 or VIF > 5), these indicators are recommended for re-evaluation, removal, or rewording to reduce multicollinearity without compromising construct coverage. After such refinement, a re-estimation is recommended to assess changes in AVE, CR, and VIF. Overall, the measurement model meets the required quality criteria for convergent validity, discriminant validity, and construct reliability. Therefore, the model is suitable to proceed to structural model (inner model) evaluation, including analyses of direct effects, mediation, and moderation using the SEM-PLS approach (Hair et al., 2021).

Table 3. SEM-PLS with *bootstraping*

	Loading factor	**AVE**	**rho_a (composite reability)**	**Cronbach's alpha**	**rho_c (composite reability)**	**VIF**
Acceptance criteria	**>0,7**	**>0,5**	**<5**	**>0,7**	**<5**	**<5**
Indicator			**Independent variable 1 (X1)**			
X1.1	0,932	0,737	0,902	0,888	0,931	3,677
X1.2	0,841					1,934
X1.3	0,938					3,839
Indicator			**Independent variable 2 (X2)**			
X2.1	0,937	0,872	0,955	0,953	0,969	4,134
X2.2	0,970					7,878
X2.3	0,960					6,387
Indicator			**Independent variable 3 (X3)**			
X3.1	0,929	0,890	0,963	0,959	0,973	3,674
X3.2	0,978					16,446
X3.3	0,976					15,755
Indicator			**Dependent variable (Y)**			
Y.1	0,906	0,590	0,827	0,790	0,880	3,430
Y.2	0,933					3,712
Y.3	0,670					1,257
Indicator			**Control variable (1)**			
K1.1	0,813	0,627	0,914	0,804	0,881	1,740
K1.2	0,790					1,618
K1.3	0,925					2,043
Indicator			**Control variable (2)**			
K2.1	0,832	0,595	0,873	0,825	0,890	2,324
K2.2	0,865					1,561
K2.3	0,867					2,195
Indicator			**Control variable (3)**			
K3.1	0,919	0,814	0,930	0,929	0,955	3,116
K3.2	0,953					4,889
K3.3	0,935					4,058
Indicator			**Mediator variable**			
Me.1	0,927	0,824	0,937	0,933	0,957	3,711
Me.2	0,953					4,821
Me.3	0,937					3,653
Indicator			**Moderating variable**			
Mo.1	0,918	0,653	0,861	0,842	0,905	2,647
Mo.2	0,895					2,484
Mo.3	0,799					1,620

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Evaluation of the Structural Model (Inner Model)

Once the measurement model met the required validity and reliability criteria, analysis of the relationships among variables in the structural model was conducted. The direction of the structural paths shows that perception of chemometrics (X1) and knowledge of chemometrics (X2) exert significant influence on chemometric competence (X3), which subsequently affects scientific analytical ability (Y). In addition to direct effects, the model also demonstrates the role of the mediator (Me), which strengthens the relationship between X2 (knowledge) and Y (analytical ability), as well as the moderator (Mo), representing learning environment support or digital literacy, which amplifies the effect of X1 on X3. These findings align with Brereton et al. (2018), who indicate that competence development is not solely driven by theoretical knowledge, but also by learning environments that facilitate the practical application of data-based analysis and artificial intelligence. The integration of cognitive understanding, practical skills, and supportive learning environments accelerates the development of 21st-century scientific analytical literacy.

Research Implications

The findings of this study emphasize the importance of integrating chemometrics into science education curricula. Students' perception and knowledge were shown to directly strengthen data analysis competence, while facility support and learning experience act as contextual factors that reinforce these relationships. From a managerial standpoint, these results can guide educators and program managers in designing data- and AI-driven learning strategies, positioning chemometric skills as core learning outcomes. The integration of coding, machine learning, and chemometric data analysis can enhance computational thinking and digital literacy among science students.

Conclusion

This study confirms that mastery of chemometrics is a key component in developing scientific analytical ability in the era of AI-based learning. The results demonstrate that positive perceptions and strong knowledge of chemometric concepts and applications significantly shape chemometric competence among students and practitioners. This competence becomes an essential foundation for processing, interpreting, and making data-driven scientific decisions. Furthermore, the study indicates that analytical ability is not only influenced by theoretical understanding but also by the capacity to apply chemometric concepts in practical scenarios. Factors such as learning motivation, digital experience, and proficiency in AI-related tools further enhance the relationship between conceptual knowledge and real-world implementation in educational and research contexts. Conceptually, the findings underline the necessity of embedding chemometrics within science education to strengthen analytical literacy and computational thinking. Such an approach better prepares learners to adapt to digital technological advancements and respond to research challenges in the era of big data and artificial intelligence. Thus, this study highlights that the development of chemometric competence depends not only on knowledge, but also on attitudes, experience, and a supportive learning environment. The multidisciplinary integration of science, statistics, and technology is crucial for innovative and adaptive science education in the 21st century.

Future studies are encouraged to expand the sample size and include respondents from more diverse disciplinary backgrounds and institutions to improve the generalizability and robustness of the findings. Involving participants from non-chemistry domains, industry sectors, and vocational education may provide a more comprehensive understanding of chemometric competence within interdisciplinary and applied contexts. Larger samples would also enable more stable estimation of complex SEM–PLS models and allow for multi-group analysis across educational levels or professional categories. In addition, future research should move beyond self-reported perceptions and knowledge by incorporating experimental, quasi-experimental, or longitudinal designs. The direct implementation of chemometrics-based learning modules, laboratory practices, or AI-assisted data analysis tasks would allow researchers to empirically assess learning outcomes, skill acquisition, and performance-based competence. Longitudinal studies could further examine how chemometric competence evolves over time in response to curriculum integration and technological exposure.Finally, subsequent studies may explore advanced modeling approaches, such as predictive-oriented SEM, hybrid SEM–machine learning frameworks, or integration with learning analytics, to strengthen the predictive and explanatory power of chemometric competence models. Such approaches would contribute to the development of evidence-based strategies for AI-driven science education and support the formulation of adaptive, data-informed curricula in higher education.

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