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## Smart Spectroscopy: AI-Driven UV Analysis for High-Throughput DNA Screening

S. Jai Surya<sup>a\*</sup>, P. Shek Abdullah<sup>a</sup>, S. Hameedul Fahim<sup>a</sup>, S. Varshini<sup>a</sup>  
S. Venuharini<sup>a</sup>, Dr. Ravisankar Mathesan<sup>a</sup>, Dr. Nataraj Palaniyappan<sup>b</sup>

<sup>a\*</sup> Srinivasan College of Pharmaceutical Sciences, Trichy

<sup>b</sup> Scientist, Novitium Pharma LLC, New jersey, USA.

\*Corresponding Author: S. Jai surya

Email Id: jai735840@gmail.com



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**Abstract:** The growing demand for rapid and reliable DNA analysis in genomics, diagnostics, and pharmaceutical research has driven the evolution of analytical technologies toward automation and intelligence. Ultraviolet (UV) spectroscopy has long served as a fundamental technique for DNA quantification and purity assessment due to its simplicity, speed, and cost-effectiveness. However, conventional UV methods are limited by their dependence on fixed absorbance values and ratio-based interpretations, which often fail to capture subtle spectral variations and complex sample interferences. The integration of artificial intelligence (AI) into UV spectroscopy has introduced a paradigm shift, enabling comprehensive spectral analysis, automated interpretation, and predictive modeling. AI-driven approaches, including machine learning and deep learning algorithms, can extract meaningful insights from full-spectrum data, enhancing accuracy and reproducibility. This review explores the concept of smart spectroscopy, focusing on AI-driven UV analysis for high-throughput DNA screening. It discusses the principles of UV spectroscopy, the role of AI in spectral interpretation, advancements in data processing, applications across various domains, and future perspectives. The convergence of UV spectroscopy and AI represents a powerful strategy for next-generation molecular analysis.

**Keywords:** Artificial Intelligence, UV Spectroscopy, DNA Analysis, High-Throughput Screening, Machine Learning, Spectral Analysis, Nanodrop, Molecular Diagnostics

### 1. Introduction

DNA analysis plays a central role in modern scientific research, forming the basis of studies in molecular biology, clinical diagnostics, forensic science, and drug development. Among the various analytical techniques available, UV spectroscopy has remained a widely adopted method for routine DNA quantification and purity evaluation due to its simplicity and rapid

analytical capability. DNA molecules absorb ultraviolet light strongly at 260 nm, enabling direct estimation of nucleic acid concentration with minimal sample preparation.<sup>1</sup> Despite its widespread use, traditional UV spectroscopy is constrained by several analytical limitations. The method relies heavily on fixed absorbance values and ratio-based interpretations, which may not accurately reflect complex sample compositions.

Contaminants such as proteins, RNA, and organic solvents often interfere with absorbance readings, leading to potential inaccuracies.<sup>2</sup> Furthermore, conventional approaches do not exploit the full spectral information available, thereby limiting analytical depth. The integration of artificial intelligence (AI) into UV spectroscopy represents a transformative advancement in analytical science. AI-driven systems enable comprehensive spectral interpretation, automated decision-making, and predictive analysis, thereby enhancing the reliability and efficiency of DNA analysis. This review examines the emerging field of smart spectroscopy, focusing on the application of AI in UV-based high-throughput DNA screening.<sup>3</sup>

## 2. Fundamentals of UV Spectroscopy in DNA Analysis - DNA Quantification and Purity Assessment

UV spectroscopy is based on the absorption of ultraviolet light by molecules, resulting in electronic transitions within the molecular structure. DNA exhibits a characteristic absorbance peak at 260 nm due to the presence of aromatic nucleotide bases. This property forms the basis for its quantification using Beer-Lambert's law, which establishes a linear relationship between absorbance and concentration under ideal conditions.<sup>4</sup> In addition to quantification, UV spectroscopy is commonly used to evaluate DNA purity through absorbance ratios such as  $A_{260}/A_{280}$  and  $A_{260}/A_{230}$ . These ratios provide indirect information about protein and organic contamination, respectively. However, such measurements are inherently simplistic and may not accurately capture the complexity of biological samples. Environmental factors, including pH and ionic strength, can further influence spectral characteristics, complicating data interpretation.<sup>5</sup> Additionally, overlapping absorbance profiles of nucleic acids and contaminants limit the specificity of traditional methods. These challenges highlight the need for advanced analytical strategies capable of extracting deeper insights from spectral data. DNA quantification and purity assessment using UV spectroscopy are fundamentally based on the interaction of ultraviolet light with nucleic acids and other biomolecules present in the sample.<sup>6</sup> The principle underlying DNA quantification is the

Beer-Lambert law, which establishes a direct linear relationship between the absorbance of light and the concentration of the absorbing species. DNA molecules exhibit a strong absorbance at 260 nm due to the presence of conjugated aromatic bases, allowing for rapid and non-destructive estimation of concentration. Under standard conditions, an absorbance value of 1.0 at 260 nm corresponds to approximately 50  $\mu\text{g/mL}$  for double-stranded DNA.<sup>7</sup> This relationship provides a convenient method for routine quantification; however, its accuracy depends on factors such as sample purity, path length, and the absence of interfering substances. In addition to quantification, UV spectroscopy enables the evaluation of DNA purity through absorbance ratio analysis. Different biomolecules absorb at characteristic wavelengths, allowing indirect identification of contaminants. The ratio of absorbance at 260 nm to 280 nm is commonly used to assess protein contamination, as proteins absorb strongly at 280 nm due to aromatic amino acids. A ratio of approximately 1.8 is generally considered indicative of pure DNA, while deviations suggest the presence of impurities such as proteins or RNA. Similarly, the absorbance ratio at 260 nm to 230 nm provides insight into contamination from organic compounds, salts, and residual extraction reagents, which typically absorb near 230 nm.<sup>8</sup> An ideal ratio in the range of 2.0 to 2.2 indicates minimal contamination. Although these spectroscopic parameters provide a rapid and widely accepted approach for evaluating DNA concentration and purity, they are inherently limited by their reliance on simplified assumptions and fixed thresholds. Overlapping absorbance profiles and environmental factors can influence spectral readings, potentially leading to inaccurate interpretations. Consequently, these traditional methods are increasingly being complemented by advanced analytical and computational techniques, including artificial intelligence, to achieve more reliable and comprehensive DNA analysis.<sup>9</sup>

## 3. Smart Spectroscopy: Concept and Evolution

Smart spectroscopy represents the integration of conventional spectroscopic techniques with advanced computational tools, particularly artificial intelligence. This approach enables the transformation of raw spectral data

into actionable insights through automated analysis and pattern recognition.<sup>10</sup> In contrast to traditional methods, which rely on predefined rules, smart spectroscopy adopts a data-driven framework that adapts to complex and variable sample conditions. The evolution of smart spectroscopy has been driven by advancements in machine learning, data processing, and computational power. Modern systems can analyse entire spectral profiles, identifying subtle variations in peak shape and intensity, and correlating these features with specific sample characteristics. This capability significantly enhances the analytical performance of UV spectroscopy, particularly in high-throughput applications.<sup>11</sup>

#### 4. Role of Artificial Intelligence in UV DNA Analysis

Artificial intelligence plays a pivotal role in enhancing the analytical capabilities of UV spectroscopy. Machine learning algorithms can be trained on large datasets of spectral information to recognize patterns associated with DNA concentration, purity, and contamination. These models provide more accurate predictions

compared to traditional methods by considering the entire spectral profile rather than isolated data points.<sup>12</sup> Deep learning techniques, particularly neural networks, offer additional advantages by enabling the analysis of complex, non-linear relationships within spectral data. These models can process high-dimensional datasets and automatically extract relevant features, reducing the need for manual intervention. As a result, they are particularly effective in identifying subtle variations that may indicate contamination or sample degradation. AI-driven systems also facilitate predictive analytics, allowing for early detection of potential issues in DNA samples. This capability enhances the reliability of downstream applications and supports proactive decision-making in laboratory workflows.<sup>13</sup>

#### 5. Data Processing and Feature Engineering

The successful implementation of AI in UV spectroscopy depends on robust data processing and feature engineering. Raw spectral data often contain noise, baseline drift, and other artefacts that must be addressed through pre-processing techniques such as smoothing, normalization, and baseline correction.<sup>14</sup>

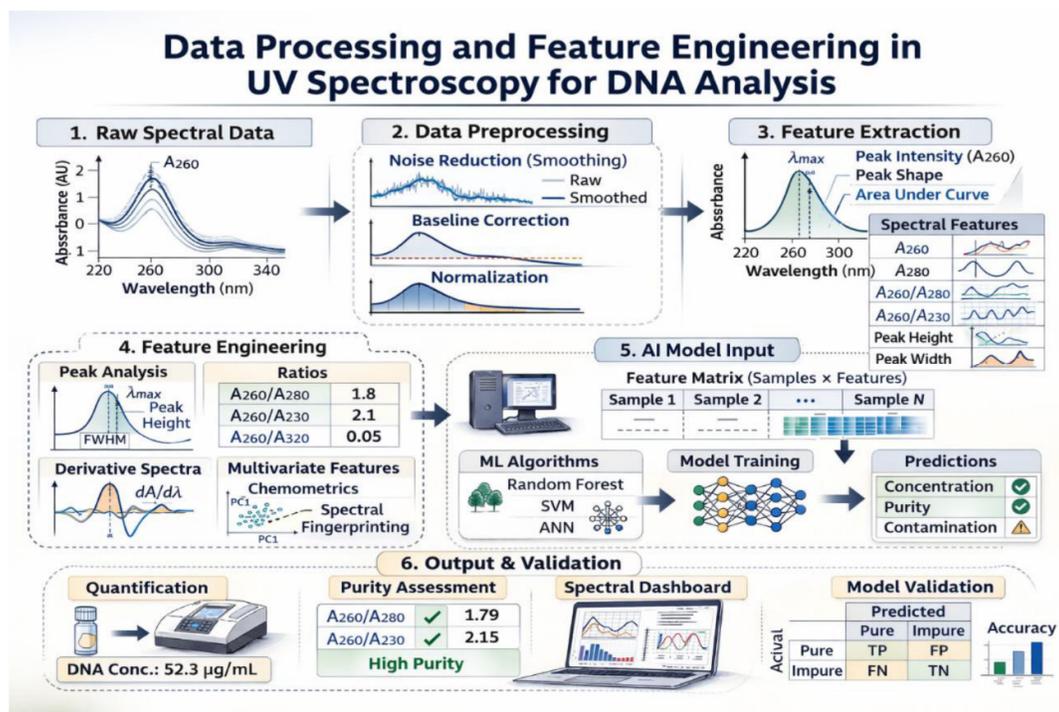


Fig 1: Data Processing and Feature Engineering

These steps are essential for improving data quality and ensuring accurate model performance. Feature engineering involves the

extraction of meaningful information from spectral data. Unlike traditional approaches that focus on specific wavelengths, AI-based methods

utilize the entire spectral range, capturing detailed information about peak shape, width, and intensity.<sup>15</sup> This comprehensive approach enhances the ability to differentiate between similar samples and detect subtle variations. Dimensionality reduction techniques, such as principal component analysis, are often employed to simplify complex datasets while retaining essential information. These methods improve computational efficiency and facilitate model training without compromising analytical accuracy.<sup>16</sup>

### 6. High-Throughput DNA Screening

High-throughput DNA screening is a critical requirement in modern research and clinical settings, where large numbers of samples must be analysed rapidly and accurately.<sup>17</sup> The integration of AI with UV spectroscopy

significantly enhances the efficiency of this process by enabling automated data analysis and interpretation. In a high-throughput workflow, samples are analysed using UV spectrophotometers equipped with automated sample handling systems. The resulting spectral data are processed by AI algorithms, which generate predictions and quality assessments in real time.<sup>18</sup> This streamlined approach reduces analysis time, minimizes human error, and ensures consistent results across large datasets. The scalability of AI-driven systems makes them particularly suitable for large-scale applications, including genomic studies and biopharmaceutical research. By automating routine analytical tasks, smart spectroscopy allows researchers to focus on higher-level data interpretation and decision-making.<sup>19</sup>

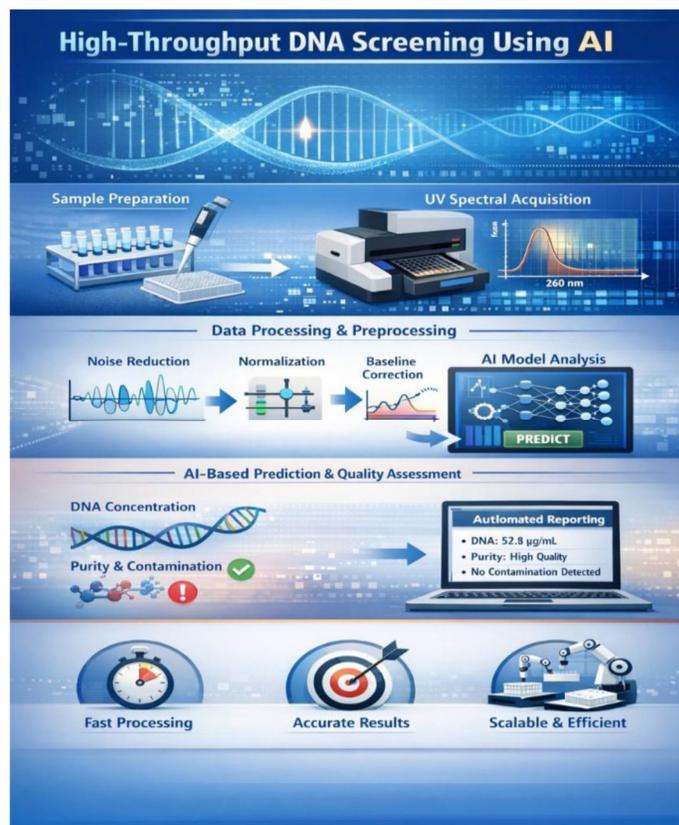


Fig 2: High-Throughput DNA Screening

### 7. Applications across Scientific Domains

The integration of AI with UV spectroscopy has broad applications across multiple scientific disciplines. In genomics, it supports rapid DNA quantification and quality assessment, facilitating high-throughput sequencing workflows.<sup>20</sup> In clinical diagnostics, it

enables accurate evaluation of patient samples, contributing to improved disease detection and management. Pharmaceutical research benefits from AI-driven UV analysis through enhanced quality control and monitoring of nucleic acid-based products.<sup>21-23</sup> This is particularly relevant in the development of gene therapies and biologics.

Forensic science also utilizes this technology for rapid and reliable DNA screening in investigative contexts.<sup>24</sup>

### 8. Challenges and Future Perspectives

Despite its advantages, AI-driven UV spectroscopy faces challenges related to data availability, model validation, and regulatory compliance. High-quality datasets are essential for training robust AI models, and insufficient data can limit model performance.<sup>25</sup> Additionally, the complexity of AI algorithms may hinder interpretability, raising concerns about transparency and reliability. Future advancements in explainable AI, cloud computing, and data sharing are expected to address these challenges.<sup>26</sup> The development of standardized protocols and regulatory frameworks will further facilitate the adoption of smart spectroscopy in clinical and industrial settings. Continued innovation in this field is likely to drive significant improvements in DNA analysis and molecular diagnostics.<sup>27-30</sup>

### 9. Conclusion

Smart spectroscopy represents a transformative approach to DNA analysis, combining the simplicity of UV spectroscopy with the analytical power of artificial intelligence. By leveraging full-spectrum data and advanced computational techniques, this approach overcomes the limitations of traditional methods and enables accurate, automated, and high-throughput analysis. The integration of AI enhances data interpretation, improves reproducibility, and provides predictive insights that support a wide range of scientific applications. As technological advancements continue, smart spectroscopy is poised to become a cornerstone of next-generation molecular analysis.

### References

1. Minhas-Khan A, Ghafar-Zadeh M, Shaffaf T, Forouhi S, Scime A, Magierowski S, et al. UV-Vis spectrophotometric analysis of DNA retrieval for DNA storage applications. *Actuators*. 2021; 10(10):246.
2. Mamede R, Pereira F, Aires-de-Sousa J. Machine learning prediction of UV-Vis spectra features of organic compounds related to photoreactive potential. *Sci Rep*. 2021; 11:23720.
3. Meza Ramirez CA, Greenop M, Ashton L, Rehman IU. Applications of machine learning in spectroscopy. *Appl Spectrosc Rev*. 2021; 56(8-10):733-763.
4. Chelvam SP, Ng AJY, Huang J, Lee E, Baranski M, Williams RBH, et al. Machine learning aided UV absorbance spectroscopy for microbial contamination detection. *Sci Rep*. 2025; 15:7631.
5. Shabbir SW, Chauhan S. A review on use of ultraviolet spectroscopy. *Innovare J Med Sci*. 2024; 12(4).
6. Campbell A. Recent developments in UV-visible spectroscopy for molecular characterization. *J Chem Pharm Res*. 2023; 15:062.
7. Ye F. Ultraviolet spectrum-based molecular precision detection. *Highlights Sci Eng Technol*. 2024.
8. Technology Networks. UV-Vis spectroscopy: principle, strengths and limitations and applications. 2023.
9. Yadav V, Ahuja T, Kharbanda H, Kumar D, Siddhanta S. Machine learning-augmented vibrational spectroscopy for DNA mutation detection. *Anal Chem*. 2025.
10. Guo K, Shen Y, Gonzalez-Montiel GA, Huang Y, Zhou Y, and Surve M, et al. Artificial intelligence in spectroscopy: advancing chemistry from prediction to generation. 2025.
11. Dijkstra AG, Tanimura Y. Correlated fluctuations in the excitation dynamics and spectroscopy of DNA. 2010.
12. Ignatova T, Balaeff A, Zheng M, Blades M, Stoeckl P, Rotkin SV. Two-color spectroscopy of UV excited ssDNA complexes. 2015.
13. Richter M, Marquet and P, González-Vazquez J, Sola I, González L. Femtosecond intersystem crossing in DNA nucleobase cytosine. 2021.
14. Brown TA. *Gene Cloning and DNA Analysis: An Introduction*. 7th ed. Wiley; 2016.
15. Sambrook J, Russell DW. *Molecular Cloning: A Laboratory Manual*. 3rd ed. Cold Spring Harbor; 2001.
16. Skoog DA, Holler FJ, Crouch SR. *Principles of Instrumental Analysis*. 6th ed. Cengage; 2014.
17. Lakowicz JR. *Principles of Fluorescence Spectroscopy*. 3rd ed. Springer; 2006.

18. Bishop CM. *Pattern Recognition and Machine Learning*. Springer; 2006.
19. Hastie T, Tibshirani R, Friedman J. *The Elements of Statistical Learning*. Springer; 2009.
20. Good fellow I, Bengio Y, Courville A. *Deep Learning*. MIT Press; 2016.
21. Brereton RG. Chemo metrics for pattern recognition. *Analyst*. 2009; 134:1380–1388.
22. Otto M. Chemo metrics: statistics and computer application in analytical chemistry. Wiley-VCH; 2016.
23. Wold S, Esbensen K, Geladi P. Principal component analysis. *Chemom Intell Lab Syst*. 1987; 2:37–52.
24. Geladi P, Kowalski BR. Partial least-squares regression. *Anal Chim Acta*. 1986; 185:1–17.
25. Lacuna Y, Bengio Y, Hinton G. Deep learning. *Nature*. 2015; 521:436–444.
26. Cortes C, Vapnik V. Support-vector networks. *Mach Learn*. 1995; 20:273–297.
27. Breiman L. Random forests. *Mach Learn*. 2001; 45:5–32.
28. Esteva A, Kuprel B, Novoa RA, Ko J, Swetter SM, Blau HM, et al. Deep learning in healthcare. *Nature*. 2017; 542:115–118.
29. Koura K, Exarchos TP, Exarchos KP, Karamouzis MV, Fotiadis DI. Machine learning applications in cancer prognosis. *Comput Struct Biotechnol J*. 2015; 13:8–17.
30. Xu R, Wang Q. Large-scale extraction of adverse drug events using NLP. *J Am Med Inform Assoc*. 2014; 21(5):848–855.