



QUALITATIVE ANALYSIS AND ITS APPLICATIONS IN FORENSIC MEDICINE: A COMPARATIVE STUDY OF FT-IR, GC-MS, AND RAMAN SPECTROSCOPY

Dr. Abdul Sattar Abdul Jabbar¹

sattaralhasany@gmail.com

Hajer Wahab Ahmed Hassan¹,

0009-0003-4160-7386:ORCID

hajarhaje961@gmail.com

Zainab Abbas Majid Salih¹

www.zenoab36@gmail.com

ORCID:0009-0009-7733-1880

Wala Saad Salman Dawood¹

ORCID:0009-0008-2620-4825

saadwala19@gmail.com

Yad Ayoub Khurshid Rashid¹

ORCID:0009-0005-5603-6672

yadayoob1@gmail.com

¹Ahmed Idrees Rashid Abdullah

ORCID:0009-0002-8220-5546

www.ahmedthsad139@gmail.com

¹Department of Forensic Evidence Sciences, College of Science,
Al-Kitab University, Kirkuk, Iraq

Corresponding Email: forensic.research@alkitab.edu.iq

Article history:		Abstract:
Received:	28 th February 2026	This paper discusses how qualitative methods of analysis have played a critical role in the development of forensic evidence science. The study will offer a comparative study of three of the most vital modern technologies: Fourier Transform Infrared Spectroscopy (FT-IR), Gas Chromatography-Mass Spectrometry (GC-MS), and Raman Spectroscopy. The paper will explore the physicochemical principles of each method, their ability to detect unknown substances such as narcotics, toxins, and explosive residues, and their strengths and weaknesses in comparison with each other regarding speed, sensitivity, and non-destructive analysis. Results show that integrative multi-technique method can severely decrease the error rates in analysis and increase the credibility of forensic evidence in a court. The research finds that no technique has been found to be universally better and that cross-validation between the techniques is necessary to achieve internationally accredited forensic quality standards
Accepted:	26 th March 2026	

Keywords: *Qualitative Analysis; Forensic Science; FT-IR; GC-MS; Raman Spectroscopy*

1. INTRODUCTION

Modern forensic science is based on the chemical analysis that is the basic instrument in determining and characterizing the unknown substances that are encountered in criminal cases. The qualitative analysis, the methodical use of scientific methods to identify the chemical identity of substances without considering their quantity, has become an essential part of the forensic laboratories throughout the world [1]. The determination of an unknown material with reasonable accuracy is the critical initial step to any quantitative determination and forms the scientific basis on which a legal process is based [3,17].

Qualitative analysis in forensic science has its historical foundations in the early nineteenth century with chemists like Robert Wilhelm Bunsen and Gustav Kirchhoff establishing the foundations of spectral analysis circa 1850-1859 in which elements could be identified by their characteristic spectral fingerprint [2]. Another major advancement was in 1910 when French criminologist Edmond Locard founded the first forensic laboratory in Lyon, France, and formulated his

groundbreaking rule: Every contact leaves a trace. This principle boosted qualitative analysis to become a forensic tool of the first order in the linking of physical trace evidence with suspects and crime scenes [3].

Modern forensic laboratories are still confronted with the same difficulty of successfully identifying the unknown chemical substances that relate to criminal cases. The scientific evidence in any court of law may be undermined by any analytical error. Although many analytical methods exist, they are all associated with some benefits and drawbacks and the primary question is, how can we be able to achieve consistent and legally acceptable qualitative findings using current analytical methods in forensic medicine? [17].

This paper will answer this question by providing a comparative analysis of three of the most popular analytical platforms: FT-IR, GC-MS, and Raman Spectroscopy assessing theoretical foundations of these methods, their practical characteristic of performance, and their application in the field of forensics. The value of this research is the integrated perspective where cross-validation of multi-techniques is offered as the gold standard of forensic qualitative analysis to reduce errors to the minimum and increase the evidentiary quality of the analytical findings.

2. LITERATURE REVIEW

Recent research has made great progress in the field of spectroscopic and chromatographic methods in the field of forensics. Skoog, Holler, and Crouch (2022) present a definitive coverage of instrumental analytical principles, which form the theoretical framework of FT-IR, GC-MS, and other techniques when applied to complex forensic matrices [1,6,9]. Their contribution emphasizes the paramount role of Michelson interferometry and Fourier transformation in facilitating fast and high-resolution infrared spectral measurements.

Houck (2023) provides an extensive list of forensic applications of FT-IR, which have been used to analyse paint fragments of traffic accidents, identify fibres, and characterise drugs, including distinguishing between hydrochloride and free-base forms of controlled substances [7]. Supplementary research by Bell (2022) discusses spectral analysis in the forensic chemistry setting, with GC-MS as the ultimate confirmatory criterion in the identification of organic compounds, especially in cases of toxicology and in arson investigations [8,11].

A systematic review of the applications of Raman spectroscopy in the field of forensic science was published in the Egyptian Journal of Forensic Sciences (2016), and it reports the increasing use of Raman spectroscopy in forensic science in the field [13]. A more recent study by Askar et al. (2025) confirmed a quick GC-MS screening procedure of seized drugs in forensic studies, showing the technique to have the ability to separate complicated mixtures in less than ten minutes with internationally recognized sensitivity limits [16].

Scholarship in the Arabic language has also had its share in this area. Al-Jader (2019) discussed the field of forensic chemistry and the ways in which it is used in investigations in Arab courts, and Al-Otaibi (2021) explored the application of spectroscopic methods in the detection of new psychoactive substances, highlighting the increased applicability of these practices to new drug threats [17,18]. Baba (2024) summarized the advances in forensic proofs based on modern scientific practices, noting that effective method validation procedures should be based on international standards [15]. Taken altogether, the literature leads to a common conclusion that, although each of the techniques presents its unique strengths, the most valid and legally justifiable analytical results can be obtained with the help of an integrative method, combining the complementary abilities of the spectroscopic and chromatographic techniques. This research is a continuation of this consensus, offering a systematic comparative system and a case-based confirmation of the integrative model.

3. METHODOLOGY AND STUDY DESIGN

3.1 Study Design

This paper is based on a systematic comparative review approach, which involves theoretical analysis of principles of instrumentality and practical assessment of the results of forensic cases. These three analytical dimensions are included in the research design: (1) theoretical-physical principles of each method; (2) practical-instrumental performance parameters such as sensitivity, selectivity, speed, and non-destructiveness; and (3) forensic usefulness of the application in actual cases of crime in the world.

3.2 Measurement Tools

The three analytical methods that are under discussion are Fourier Transform Infrared Spectroscopy (FT-IR), utilizing Michelson interferometry and Fourier transformation to create molecular fingerprint spectra at 4000-4000 cm⁻¹; Gas Chromatography-Mass Spectrometry (GC-MS), which combines capillary column separation with electron ionization mass spectrometry (70 eV standard) and NIST

3.3 Data Collection Procedures

The peer-reviewed articles published in 2019-2025 were gathered as performance data, and the forensic cases were documented to ensure that the information received via international court proceedings is supported with the help of the peer-reviewed articles. The key parameters put into consideration included: limit of detection (LOD), analytical specificity, sample preparation, analysis time, portability, applicability in courts of law, and cost relative. The comparative structure was pre-designed in such a manner that the direct cross-technique evaluation could be carried out in the following parameters..

3.4 Statistical and Analytical Approach

As this research is qualitative-comparative, the performance data are provided in organized tabular form that facilitates a systematic comparison with cross-techniques. The outcomes of cases in forensics are evaluated through a narrative analysis in relation to the outcomes of evidence and judicial acceptance. The integrative analytical model is compared with the international quality standards such as ISO/IEC 17025 requirements on forensic laboratory competence..

4. RESULTS AND DISCUSSION

4.1 FT-IR: Principles, Performance, and Forensic Applications

Fourier Transform Infrared Spectroscopy is based on the principle that the molecular bonds absorb infrared radiation at characteristic frequencies that depend on atomic mass and strength of bonds, creating a distinctive spectral fingerprint of each chemical compound [5]. All frequencies are collected by the Michelson interferometer at the same time, and converted out of the time domain and into the frequency domain using Fourier transformation- a process that provides better signal-noise ratio than other dispersive instruments [1].

The region of paramount forensic significance is the fingerprint region ($400\text{-}1500\text{ cm}^{-1}$) which harbors the complex vibrational patterns which are indicative of the entire molecular structure such that it is practically impossible to have two structurally different compounds give the same spectra in the fingerprint region [2]. A unique device that has had a groundbreaking effect on the practice of forensics has been the Attenuated Total Reflectance (ATR) accessory, which allows solid and liquid samples to be examined directly without destructive preparation of the samples, retaining exhibit integrity to further analysis [7].

FT-IR has been used in forensic drug analysis to differentiate chemically similar drugs (e.g., cocaine hydrochloride and crack cocaine free base) and to detect cutting agents (e.g., starch and lactose) at the same time [7]. Micro-FT-IR analysis of paint transfer evidence, cross-referenced to the international database of Paint Data Query (PDQ), can be used in traffic accident investigations to identify vehicle makes and models using microscopic pieces of paint [7]. The method is also used in the examination of documents, analysis of inks and the analysis of chemical contaminants in food and liquid samples [8].

One of the pioneering uses of FT-IR fiber analysis was in the Ted Bundy serial murder cases (United States, 1970s-1980s), in which infrared spectroscopy confirmed that fibers found at the bodies of the victims related to polymeric material in carpet samples at the suspect residence. This piece of evidence although a part of an overall evidentiary model helped the prosecution present its case and demonstrated the effectiveness of the technique in creating material connections between crime scenes and suspects [7,8].

4.2 GC-MS: Principles, Performance, and Forensic Applications

Gas Chromatography-Mass Spectrometry is universally accepted as the gold standard used in confirmatory identification of volatile and semi-volatile organic compounds in forensic matrices [9]. The method works in two steps: the gas chromatograph isolates mixture components through a difference in the way the different compounds partition through a mobile carrier gas (usually helium) and a stationary phase layer coating the capillary column whereas the mass spectrometer disintegrates ionized molecules and sorts the fragments of ions by mass-to-charge ratio (m/z) [9,10].

Dual-identification mode of GC-MS, retention time and mass spectral fragmentation pattern allow the probability of misidentification to be near to zero even with a very complex matrix [9,11]. The electron ionization of the standardized 70 eV potential creates reproducible fragmentation patterns that can be compared to the NIST Mass Spectral Library with more than 350,000 reference spectra, which offer courts an internationally validated system of identification [11]. Capillary column technology has also developed modern technology that has decreased the time of analysis of complex mixtures down to less than ten minutes, a major breakthrough to the operational forensic laboratories [16].

A prominent application of GC-MS in forensic history was given in the 1982 Chicago Tylenol Murders case. After several people died after taking cyanide-contaminated Tylenol pills, GC-MS testing showed the presence of fatal cyanide levels with mass spectral pattern matching, proving the cause of death and leading to the wholesale restructuring of pharmaceutical packaging safety regulations in the United States [10,11].

In the anti-doping of sport, the GC-MS analysis of urine samples of Canadian sprinter Ben Johnson in the 1988 Olympics at Seoul revealed the banned anabolic steroid stanozolol in parts per billion (ppb), which caused him to lose his Olympic medal. This case established GC-MS as the absolute method of anti-doping analysis and it proved the method to have an unprecedented sensitivity in detecting trace organic compounds [10,11].

4.3 Raman Spectroscopy: Principles, Performance, and Forensic Applications

Raman Spectroscopy In 1928, Indian physicist C.V. Raman described the elastic scattering of monochromatic laser light by molecular vibrations, which has become known as Raman Spectroscopy [18]. When laser photons contact a sample, the huge majority of them scatter elastically (Rayleigh scattering) without any photon energy change; a minor fraction, however, couple to energy exchanges with molecular vibrational modes, emitting Raman-shifted photons with a photon energy difference that is a fingerprint of the vibrational state of the molecule [12].

Raman spectra can be described as wavenumber (cm^{-1}) shifts of excitation frequency and reflect the individual chemical bond vibrations of the analyte and provide a molecular fingerprint characteristic of a particular compound [12]. The most notable benefit of Raman spectroscopy in forensics is the fact that samples of any type can be examined using transparent packaging materials without the need to open the containers, which significantly minimizes the exposure of the operator to potentially dangerous chemicals [13]. Expansion of portable handheld Raman instruments has gone further to give the technique field deployment at crime scenes so that real-time in-situ identification can be done [13]. After the July 7, 2005 bombings in London, the use of portable Raman instruments at the blast locations was introduced in order to examine the bomb residues of the home made explosive devices. The explosives were identified as triacetone triperoxide (TATP), an organic peroxide that is manufactured using commercially available precursors. This quick identification of the field led investigators to the procurement networks of the precursor chemicals and played a key role in the further investigation [13].

Raman spectroscopy has played a conclusive role in realising or disproving artworks by Pablo Picasso in the field of art forensics. The study of pigments in suspected forgeries showed that they contained synthetic pigments that were not commercially accessible at the time Picasso was alive, and gave conclusive chemical evidence of inauthenticity. This application is an example of the wide implications of Raman spectroscopy in economic and cultural heritage crime on top of conventional criminal forensics [14].

4.4 Comparative Performance Analysis

Table 1 provides a comparative system of the three analytical methods in terms of the major performance and forensic application parameters.

Table 1: Comprehensive Comparison of FT-IR, GC-MS, and Raman Spectroscopy in Forensic Applications

Parameter	FT-IR	GC-MS	Raman Spectroscopy
Working Principle	IR absorption by molecular bonds	Gas separation + mass fragmentation	Inelastic laser light scattering
Sample Types	Solid, liquid, gas	Volatile/semi-volatile compounds	Solid, liquid, powder
Sensitivity	Moderate to high	Very high (ppb level)	Moderate to high
Selectivity	High (spectral fingerprint)	Very high (gold standard)	High (molecular fingerprint)
Sample Destruction	Non-destructive (ATR)	Partial vaporization (requires)	Non-destructive
Analysis Time	10–30 minutes	Minutes to 30 minutes	Seconds to minutes (portable)
Field Deployment	Limited	Not available	Yes (portable devices)
Relative Cost	Moderate	High	Moderate to high
Court Acceptance	High	Very high (gold standard)	High
Key Applications	Fibers, paints, drugs, documents	Toxins, stimulants, explosives, arson	Explosives, drugs, ink, art forgery

The comparative analysis shows that both techniques have a different and complementary niche of analysis. FT-IR offers quick non-destructive, molecular fingerprinting best suited to both solid and liquid trace material. The confirmatory power of GC-MS in volatile organics is unsurpassed, and identification on a court-acceptable basis of matching mass spectral library and dual retention time is possible. The special capability of non-destructive through-packaging field analysis is found only in Raman spectroscopy, giving it the advantage of being used over initial scene assessment and a screen of hazardous materials [19].

The data effectively embrace the integrative analytical model whereby FT-IR or Raman spectroscopy is conducted to screen the data, and GC-MS is conducted to give a confirmatory identity. The sequential protocol reduces instances of false identification and maximizes resource use as well as preserving the chain of custody integrity needed to ensure that evidence is admissible.

5. CONCLUSION

This paper has affirmed that qualitative analysis in forensic science has indeed risen above being a standard laboratory process to form a scientific system that is part and parcel of criminal justice today. The proper chemical identification of unknown substances is not only a technical achievement, but it is the scientific limit of reasonable doubt and judicial certitude.

The three methods discussed- FT-IR, GC-MS, and Raman Spectroscopy are complementary levels of analytical performance ascending in order of speed screening spectroscopic to high-selectivity confirmatory analysis. The real forensic worth of these platforms is not the preeminence of any individual technique, but the ability to operate as part of an integrative protocol of analysis that offers results verification with each other and reduces the possibility of error.

Based on the findings, the following recommendations are advanced:

- All three analytical platforms of FT-IR, GC-MS, and Raman Spectroscopy should be positioned in the forensic labs but not in isolation.
- Preliminary screening with FT-IR or Raman should be a standard procedure in the analytical protocols, with mandatory confirmation by GC-MS before final reports are produced in legal cases.

- Portable Raman instruments should also be supplied to be used in the field during crime scenes to facilitate preliminary identification in real-time.
- Forensic analysts are supposed to have thorough training in the interpretation of the results in line with the international standards of result interpretation (ISO/IEC 17025), where proficiency testing is conducted regularly.
- Laws need to be drawn to provide a set standard of admissibility of spectroscopic and chromatographic evidence such as the standard validation of methods before official use.
- Reference spectral databases must be updated on a continual basis to cover new controlled substances and new psychoactive materials.

REFERENCES

- [1] Skoog, D. A., Holler, F. J., & Crouch, S. R. (2022). *Principles of Instrumental Analysis* (8th ed.). Cengage Learning.
- [2] Silverstein, R. M., Webster, F. X., & Kiemle, D. J. (2014). *Spectrometric Identification of Organic Compounds* (8th ed.). Wiley.
- [3] Rhodes, H. T. F. (1956). *Alphonse Bertillon: Father of Scientific Detection*. Abelard-Schuman.
- [4] Bell, S. (2022). *Forensic Chemistry* (3rd ed.). Pearson.
- [5] Silverstein, R. M., Webster, F. X., & Kiemle, D. J. (2014). *Spectrometric Identification of Organic Compounds—Chapter: IR Spectroscopy*. Wiley.
- [6] Skoog, D. A., Holler, F. J., & Crouch, S. R. (2022). *Principles of Instrumental Analysis—FT-IR Chapter*. Cengage Learning.
- [7] Houck, M. M. (2023). FT-IR Applications in Forensic Science. In *Fundamentals of Forensic Science* (4th ed., pp. 210–235). Academic Press.
- [8] Bell, S. (2022). Spectral Analysis Techniques in Forensic Chemistry. In *Forensic Chemistry* (3rd ed., pp. 180–205). Pearson.
- [9] Skoog, D. A., Holler, F. J., & Crouch, S. R. (2022). Gas Chromatography and GC-MS. In *Principles of Instrumental Analysis* (8th ed., pp. 850–910). Cengage Learning.
- [10] Houck, M. M. (2023). Advances in Capillary Columns and GC-MS Applications. In *Fundamentals of Forensic Science* (4th ed., pp. 260–290). Academic Press.
- [11] Bell, S. (2022). GC-MS as Legal Evidence and NIST Library Matching. In *Forensic Chemistry* (3rd ed., pp. 220–248). Pearson.
- [12] Silverstein, R. M., Webster, F. X., & Kiemle, D. J. (2014). Raman Spectroscopy. In *Spectrometric Identification of Organic Compounds* (8th ed., pp. 95–120). Wiley.
- [13] *Egyptian Journal of Forensic Sciences*. (2016). Review on Raman Spectroscopy applications in forensic science. *Egyptian Journal of Forensic Sciences*, 6(3), 209–215.
- [14] Houck, M. M. (2023). Raman Spectroscopy in Field Investigations. In *Fundamentals of Forensic Science* (4th ed., pp. 310–325). Academic Press.
- [15] Baba, M. T. (2024). Forensic proof using modern scientific methods. *Journal of Human and Natural Sciences*, 6(9), 705–765. <https://doi.org/10.53796/hnsj69/45>
- [16] Askar, A. M., Al Ali, A. Y., Khalifa, M. K., Salem, A. A., Alkhuwaildi, B. M., & Shah, I. (2025). Rapid GC-MS method for screening seized drugs in forensic investigations: Optimization and validation. *Forensic Science International*, 356, 112301. <https://doi.org/10.1016/j.forsciint.2024.112301>
- [17] Al-Jader, W. A. (2019). Forensic chemistry and its applications in criminal investigation. *Journal of Babylon University for Pure and Applied Sciences*, 27(2), 1–15.
- [18] Al-Otaibi, M. S. (2021). Use of spectroscopic analysis techniques in the detection of novel psychoactive substances. *Arab Journal of Forensic Sciences and Forensic Medicine*, 3(1), 45–62.
- [19] Arab Organization for Administrative Development. (2020). *Guide to forensic laboratories in Arab countries*. Cairo: League of Arab States.