SHIMADZU
Excellence in Science

Analytical Instruments

Solutions for Seized Drugs

When it comes to the analysis of seized drug samples, each laboratory is responsible for properly analyzing a material as it pertains to a court of law and prosecution. Materials can come in a variety of forms, such as powder, pills, tablets, e-liquids, oils and even edibles. The Scientific Working Group for the Analysis of Seized Drugs (SWGDRUG) and the Organization for Scientific Committees (OSAC) for Forensic Science provide the minimum requirements for the development of an analytical scheme for proper identification of a drug or chemical. Shimadzu offers a series of analytical tools for a forensic chemist to accurately identify and confirm a controlled substance based on levels of selectivity.

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Category C

Fluorescence Spectroscopy

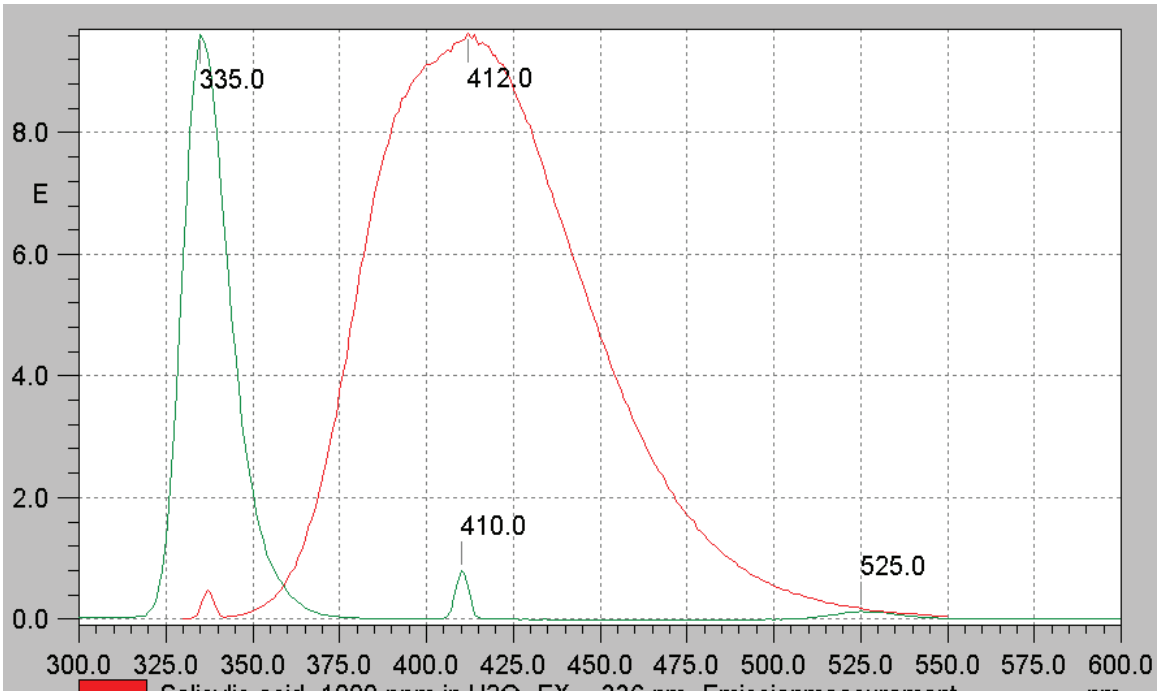
This technique can detect a compound based on its fluorescent properties. While not all compounds fluoresce, those that do are unique. It is considered to have the lowest level of selectivity and is one technique that is used for screening of drug samples.

Fluorescence Spectrofluorometer
RF-6000

Delivering high speed, stability and sensitivity, the RF-6000 offers the ultimate performance for both routine and challenging applications. Outstanding sensitivity and a market-leading signal-to-noise ratio allow for very low limits of quantitation, while high-speed 3D scanning of 60,000 nm/min enables acquisition of a 3D fluorescence spectrum in a very short time, with individual scans acquired in just one second. An extended upper wavelength range to 900 nm ensures measurements of substances that exhibit fluorescence at longer wavelengths.

User-friendly LabSolutions RF software features sophisticated, yet easy-to-use functionality ranging from standard fluorescence to 3D measurements of fluorescence spectra at any wavelength interval.

Generating a library of emission and excitation spectra for compounds and impurities found in dry samples allows for an initial compound classification before further analysis by a more selective technique. Here we show an example of the emission and excitation spectra from salicylic acid.



Emission spectrum (red) and excitation spectrum (green) from salicylic acid, 1000ppm in H_2O

Category B

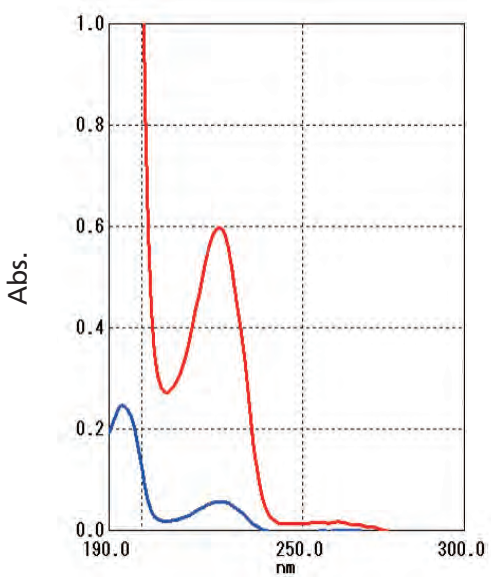
UV-Vis Spectroscopy

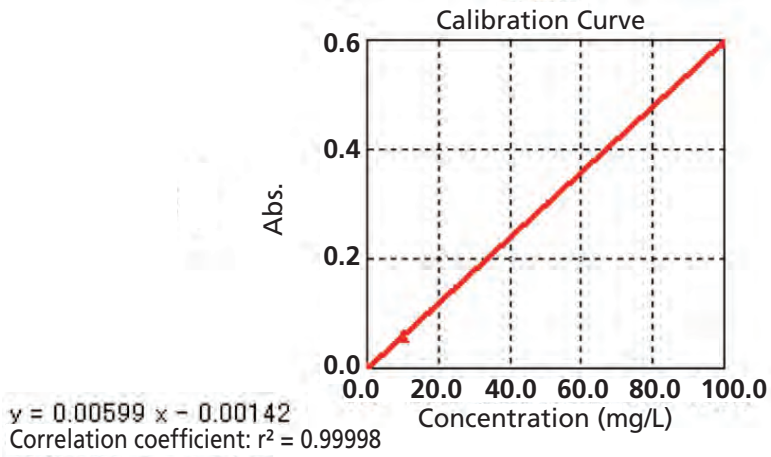
Often used as a preliminary test to identify unknown compounds for further testing, UV-Vis spectroscopy measures the absorption of light in the ultraviolet-visible spectral region.

UV-Vis Spectrophotometer
UV-1900i

Shimadzu's workhorse UV-1900i spectrophotometer incorporates advanced features that improve usability, regulatory compliance, and performance, making it ideal for the forensics lab. It features high resolution, low stray light, high reproducibility, and an ultra-fast scan function, while the easy-to-use interface simplifies operation and enables acquisition of results quickly and easily.

LabSolutions UV-Vis software features a simple design layout that enables even first-time users to perform operations easily. Numerous functions, including data transfer to spreadsheet software and batch text export of multiple data sets, significantly enhance the efficiency of routine analysis.





The figure on the left shows the absorption spectrum of detergent A. The sample concentrations are 100 mg/L (red) and 10 mg/L (blue). The figure on the right shows the calibration curve at a measurement wavelength of 225 nm. These results illustrate the method of calculating quantitation limits based on measurements conducted using an UV-Vis spectrophotometer.

Determination of the quantitation limit makes it possible to verify the lower limit of residual substances and residual detergent that can be quantitated.

Category B

Gas Chromatography

Seized materials have to be properly identified to determine if they contain controlled substances as described in the Controlled Substances Act (CSA). Gas Chromatography (GC) has been the gold standard for separation and analysis of seized materials in forensic labs for many years due to its robustness and efficient results. This section will describe GC separation using flame ionization detection (FID) for analysis of common seized drugs and chemicals.

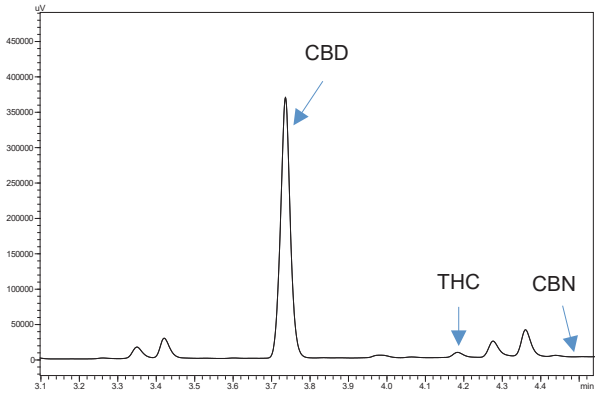
Gas Chromatograph
Nexis GC-2030

The Nexis GC-2030, Shimadzu's premier gas chromatograph, offers a modern approach to a classic chromatographic technique. Designed with the user in mind, new innovative features, exceptional performance, high-throughput capabilities and a variety of inlets and detectors will elevate your lab to the next level. An integrated hydrogen sensor option allows use with hydrogen carrier gas.

Analysis of THC and CBD Content in Hemp Oil

The Hemp Farming Act of 2018 removes the plant Cannabis Sativa L. from the controlled substances act if it contains no more than 0.3% THC on a dry weight basis. It is important to accurately distinguish hemp from cannabis using a quantitative analysis of the material.

Hemp oil containing beneficial phytocannabinoids such as cannabidiol (CBD) but very low levels of the psychoactive compound tetrahydrocannabinol (THC) has become increasingly popular. In order to comply with the Hemp Farming Act of 2018, the levels of CBD and THC should be closely monitored. Shown here is data from an analysis using a GC-2030 with FID.



Analysis of Structural Isomers using GC-VUV

Using ultraviolet spectroscopy detection, one can differentiate diastereomers of common controlled substances that are not separated using other analysis techniques.

Category B

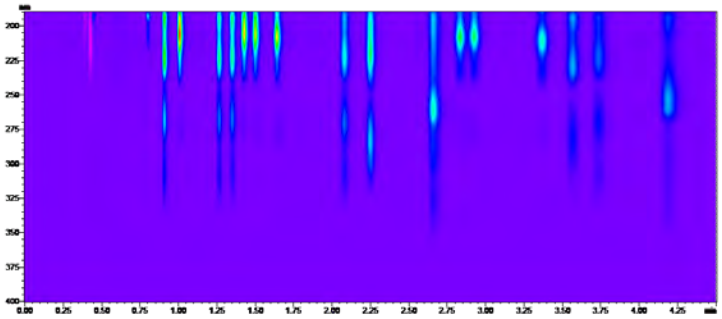
Liquid Chromatography

Traditionally, liquid chromatography (LC) has not been the most common separation technique used for the identification of seized drugs, but with the passing of the Hemp Farming Act in 2018 and the need for faster analysis, it is being adopted in more crime laboratories. Compounds that may not separate well using GC techniques are able to be fully resolved using LC. LC can completely separate compounds in their native form. With GC, some compounds like THC-A will decompose in the heated inlet. In addition, the need for derivatization of certain compounds is eliminated when using LC techniques.

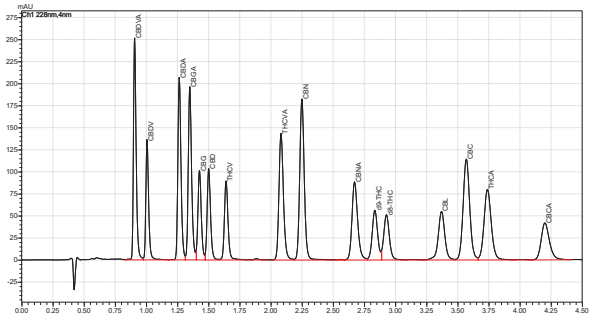
Cannabis and Hemp Analyzers

Shimadzu's Cannabis and Hemp Analyzers are the comprehensive solutions for cannabinoids analysis, providing accurate results with minimal effort to quantitate THC. Traditional HPLC with UV-Vis detection is the gold standard for cannabinoids analysis, including the acidic forms; however, using a photodiode array (PDA) detector instead of a UV-Vis detector allows recording of the full absorption spectrum from 190-400 nm.

Here is an example separation of 16 cannabinoids by UHPLC-PDA in under 5 minutes.

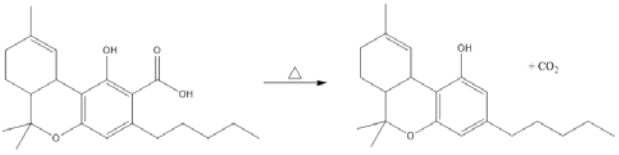


Analysis of 16 Cannabinoids with the Shimadzu Nexera-i (LC-2040C 3D) UHPLC with PDA

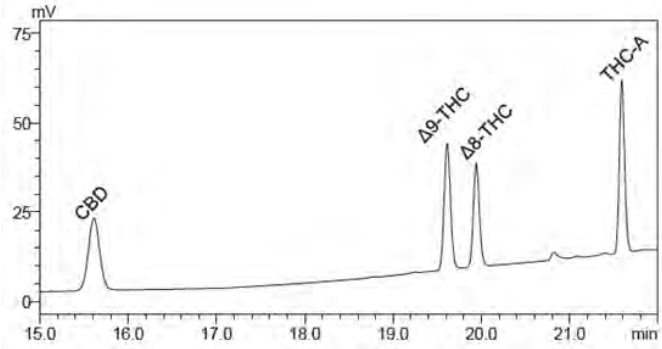


4.5 minute separation of 16 Cannabinoids by UHPLC-PDA

Additionally, when distinguishing between hemp and cannabis, it is important to have complete resolution of tetrahydrocannabinol (psychoactive component) and its analogs: Δ8-THC, Δ9-THC, THC acid and CBD. Shown here is an example of a separation with baseline resolution of these four compounds.



Decarboxylation of THC-A to THC



Category B

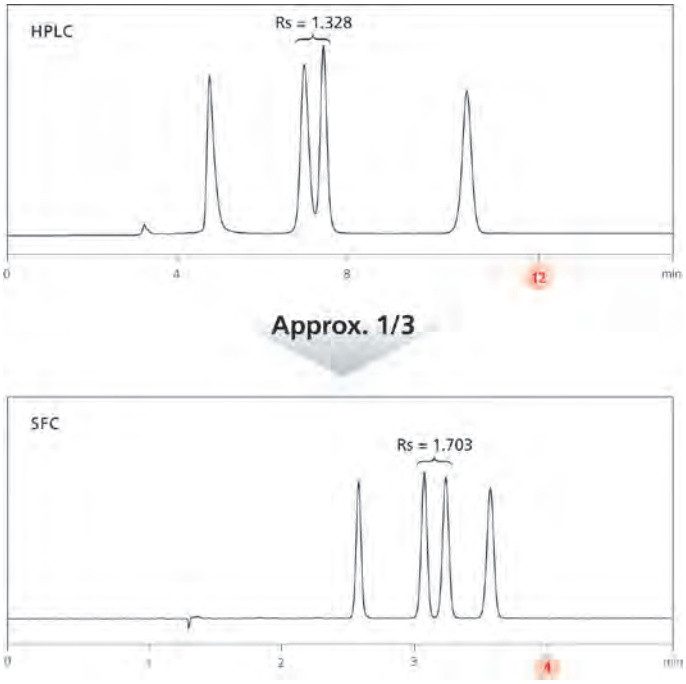
Supercritical Fluid Chromatography

Supercritical fluid chromatography (SFC) is another separation technique that uses supercritical carbon dioxide as a mobile phase. SFC provides a fast separation of isomeric and chiral compounds, such as D and L amphetamine, with improved peak capacity and chromatographic resolution. The power of SFC is in its alternate, often unique selectivity.

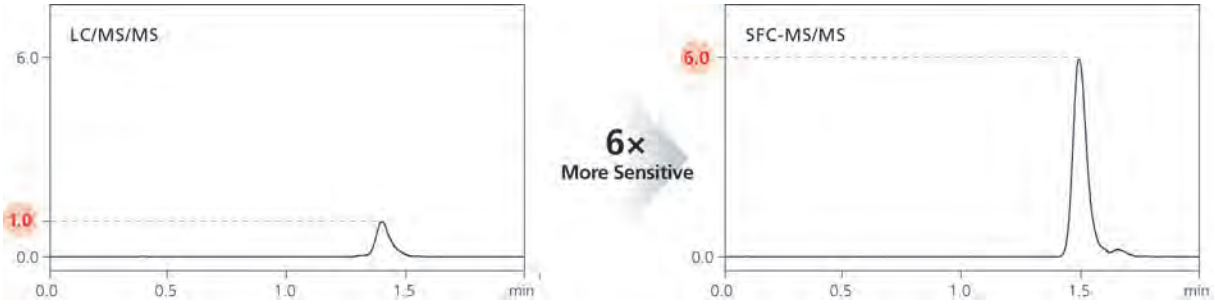
Supercritical Fluid Chromatograph
Nexera UC

The Nexera Unified Chromatography (UC) system provides efficient separation of analogues or chiral compounds with higher sensitivity and resolution than traditional LC. In addition, it helps to minimize environmental impacts and costs by reducing the amount of organic solvents needed.

Improved separation and detection capabilities result from the low viscosity and high diffusion coefficient of supercritical fluid. As shown below, Nexera UC demonstrates high separation selectivity for isomeric compounds that are difficult to separate by conventional LC.



In addition, using SFC as the front end for a mass spectrometer offers greater sensitivity than achieved with LC-MS/MS.



Category A

Gas Chromatography-Mass Spectrometry

Mass spectrometry offers the highest level of selectivity for compound identification. Having the ability to obtain mass confirmation data aids in the verification of the drug or chemical. The most common technique used for qualitative analysis of drugs or substances, gas chromatography mass spectrometry (GC-MS) produces a chemical fingerprint based on mass that is unique to each compound or substance.

Gas Chromatograph Mass Spectrometer: GCMS NX Series with Autosampler

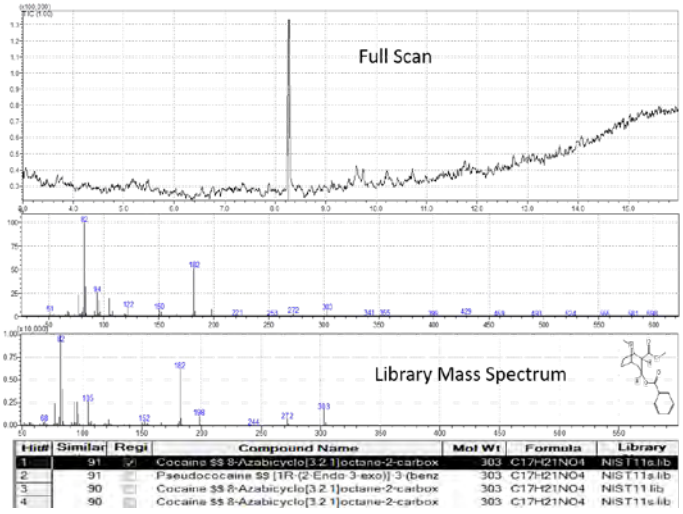
Utilizing the most advanced gas chromatograph available, and incorporating a variety of technological advances, Shimadzu's NX series of single-quad GC-MS instruments offers the highest performance levels available. In addition to outstanding functionality, they come equipped with a variety of Smart features, easy maintenance, and intuitive software, enabling efficient workflows, greater uptime, and reduced costs for higher productivity and better ROI.

Combine a GC-MS system with the AOC-20i auto injector or the AOC-6000 robotic autosampler for ideal sample handling with high throughput, data reliability and traceability.

Analysis and Quantitation of Cocaine on Currency

Paper currencies around the world are usually made of a cellulose-based paper which can adsorb cocaine onto the surface, and when a person handling cocaine subsequently touches paper money or uses the bill as a tool to inhale cocaine, the currency easily becomes contaminated. When this contaminated paper money comes into contact with other bills, the cocaine is easily transferred from one bill to the next.

In this example, a GC-MS analysis method for cocaine was quickly and easily developed at point-of-use. The GC-MS was used to create a calibration curve for cocaine and results were confirmed with the NIST/Wiley library. Fifteen individual paper currency notes from multiple countries were analyzed and quantitated (ng) for cocaine.



Full-scan TIC of Cocaine with Spectrum and Library Search Results

Origin of Currency Tested	Denomination	Amount of Cocaine Found
USA, Florida	20 Dollars ($20)	1.76 ng
USA, Florida	20 Dollars ($20)	8.25 ng
USA, New Jersey	1 Dollar ($1)	2.85 ng
USA, New Jersey	1 Dollar ($1)	19.6 ng
USA, New Jersey	1 Dollar ($1)	1.1 ng
China	10 Yuan	0.84 ng
Indonesia	1 Rupiah	0.68 ng
France	10 Euro	ND
Brazil	1 Real	ND
Mexico	1 Peso	ND
Mexico	10 Peso	ND
Canada	1 Canadian Dollar	ND
Britain	5 Pounds	ND
India	100 Rupee	ND
India	500 Rupee	0.69 ng
ND = Not Detected		

Amount of Cocaine Detected on Currency from Different Countries

Category A

Liquid Chromatography-Mass Spectrometry

While GC-MS remains the most common technique in the forensics lab, liquid chromatography mass spectrometry (LC-MS) has gained more acceptance in recent years. LC-MS uses a soft ionization technique to increase confidence in identification of the compound of interest by its unique mass. In comparison to GC-MS, LC-MS offers faster detection rates and an LC-MS method enables a larger drug panel to be screened simultaneously, helping to alleviate any casework backlogs. The need for a derivatization step could also be avoided.

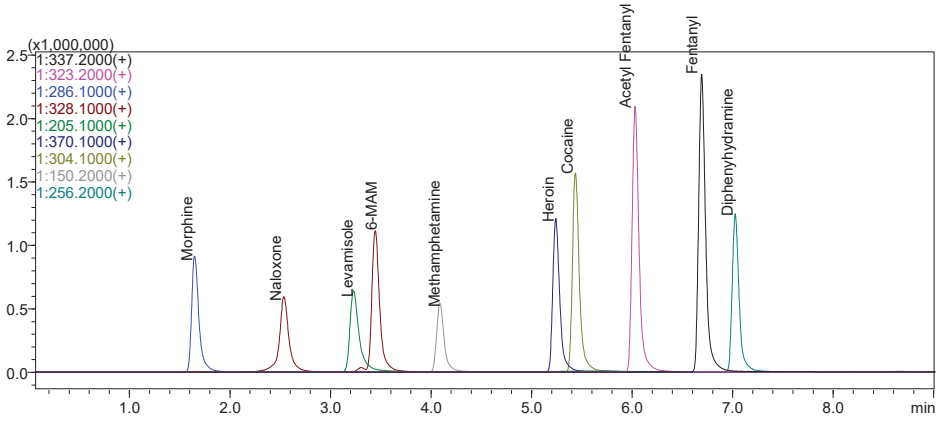
Liquid Chromatograph Mass Spectrometer LCMS-2020

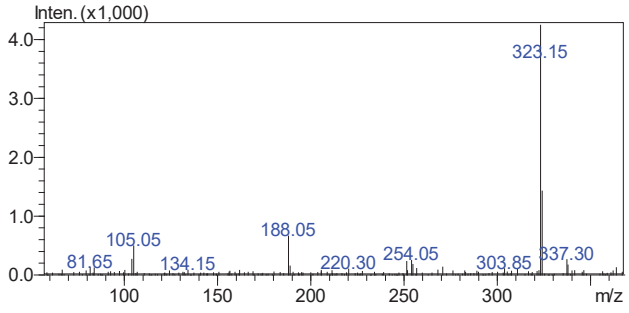
An ultra-fast single-quadrupole mass spectrometer designed for ease of use with an HPLC or UHPLC system, the LCMS-2020 offers high performance at a low cost. With its scanning speed of 15,000 u/sec, a 15 msec polarity switching speed, exceptional detection capabilities, and easy system maintenance, the LCMS-2020 enables quicker and more accurate detection of trace impurities in a variety of applications.

Identification and Confirmation of Ten Common Seized Drugs

The utilization of in-source CID allows one to acquire a unique fragmentation pattern for each compound that can be used to create a library for simple identification of unknown samples. Shown here is a representative SIM chromatogram for 10 common seized drugs at 1ug/mL and a spectrum from a scan event with 60V in-source CID for acetyl fentanyl.

Simultaneous quantitation can be performed on each compound, if that is needed for the casework.





Category A

Infrared Spectroscopy

Fourier transform infrared (FTIR) spectroscopy provides the highest level of selectivity through structural information, using the absorption of infrared radiation to produce chemical fingerprints of substances based on chemical bonds. When coupled with attenuated total reflectance (ATR), this technique is used to identify unknown powders, pills, and tablets from seized material.

FTIR Spectrophotometer
IRSpirit / IRAffinity-1

About the footprint of a typical ink jet printer, Shimadzu's IRSpirit features a small, space-saving design with the widest sample compartment in its class. It can be equipped with a variety of accessories, including ATR accessories and the SurveyIR™ microscope, making it an ideal, easy-to-use system for contaminant analysis, identification tests, and quantitative measurements. If a more powerful microscope is required, combine the IRAffinity-1 with the AIM-9000 infrared microscope. This powerful configuration simplifies micro analysis with a 30,000:1 S/N ratio, automatic contaminant recognition, and optional wide field camera.

SurveyIR™
FT-IR Microspectroscopy

The affordable SurveyIR™ microscope enables FTIR microscopy in a compact design when mounted in the sample compartment of an FTIR spectrometer. This type of infrared microscopy system is capable of measurements on minute objects down to approximately 100 µm. Infrared spectra are detected using the FTIR system's standard detector.

The SurveyIR™ is capable of transmission, reflectance, and ATR measurement (diamond or Ge prism), and an aperture can be selected from six sizes (2000, 250, 200, 160, 100, 60 µm). Therefore, measurement of minute areas is possible using SurveyIR™ if the sample is approximately 100 µm in size.

Category A

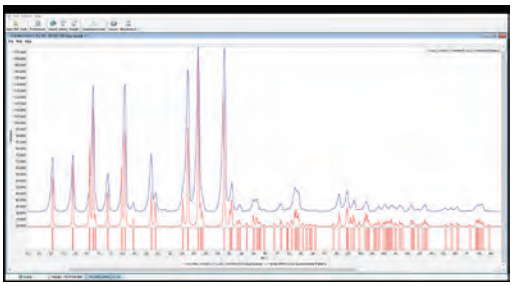
X-ray Diffractometry

X-ray powder diffraction (XRD) is an analytical method that is primarily used for phase identification of unknown powders. In addition to phase identification, the technique can be used to quantify phase, measure unit cell dimensions, and measure molecular structures. Samples are typically finely ground and homogenous.

X-ray Diffractometer
XRD-6100 / 7000

Shimadzu XRDs can be customized with different X-ray tubes, come with a high-stability X-ray generator, and complete control, analysis, and reporting software. The XRD-6100 features a Θ-2Θ goniometer design while the XRD-7000 is in the Θ-Θ configuration. The XRD-7000 includes options to accommodate samples up to 400 mm in diameter. Both the 6100 and 7000 can be equipped with the state-of-the-art OneSight detector. This detector is a silicon strip detector with 1280 channels, significantly increasing scan speed times compared to a conventional 0-D scintillator detector.

Shimadzu XRDs can be paired with ICDD PDF software, which helps facilitate rapid phase identification of bioactive, pharmaceutical and toxicological agents. In PDF-4 Organics, there are over 538,500 entries that can be compared to experimental patterns. A combination of integrated data mining software, search filters and search-matching algorithms helps enable successful, rapid identification of unknown powders.

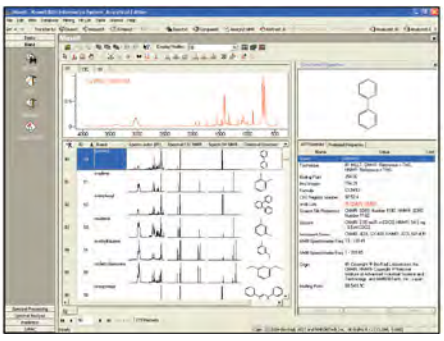


XRD pattern of Tylenol (blue trace) compared to a theoretical pattern. Courtesy of ICDD PDF-4 Organics.

Drug Libraries

Drug libraries are important for comparing spectra from unknown samples to reference spectra to increase the chance of confirming the identity of unknowns. Shimadzu offers a series of drug libraries for GC-MS, FTIR and LC-MS products.

Drug Libraries
GC-MS, FTIR, LC-MS



IR Libraries

Shimadzu offers a variety of libraries to simplify your infrared analysis of seized drugs.

- These include the SWGDRUG infrared library, generated by the Drug Enforcement Administration's Special Testing and Research Laboratory
- Wiley's KnowItAll IR Spectral Library. Offering access to over 264,000 infrared spectra, the KnowItAll IR Spectral Library for ATR-IR, FT-IR, and NIR enables cost-effective identification of unknown spectra.

GC-MS Libraries

- NIST/Wiley 11th Edition Mass Spectral Library which includes over 1 million EI mass spectra with over 770,000 unique compounds
- Designer Drugs MS Library which includes over 13,000+ GC-MS spectra for designer or medicinal drugs, CWAs and explosives.

LC-MS Libraries

- LC-MS^n Library of Drugs, Poisons and Their Metabolites library consists of over 2250 parent compounds with over 3600 metabolites.

Consumables

Shimadzu has provided over 140 years of simplicity, elegance, and innovation to the scientific community, becoming the brand researchers trust. We have developed an extensive portfolio of the highest quality consumable products to ensure your work progresses effortlessly. Whether you need new columns for liquid or gas chromatography, isotopically labeled standards for mass spectrometry work, a leak detector for a gas chromatograph, syringes, filters, and vials for sample preparation, or one of hundreds of other laboratory consumables, Shimadzu has the solution.

Table of Analytical Instruments for Forensic Applications

	Toxicology - Screening	Toxicology - Confirmation/ Identification	Toxicology - Quant	Trace Evidence (Hairs/Fibers/ Paints/Arson)	Controlled Substances/Seized Drugs
GC		✓	✓		✓
GC-MS	✓	✓	✓	✓	✓
HS GC		✓	✓		
HS GC-MS		✓	✓		
Pyrolyzer GC-MS				✓	
FTIR				✓	✓
IR Microscope				✓	✓
UV-VIS				✓	✓
Fluorescence				✓	✓
SFC					✓
LC					✓
LC-MS Single Quad	✓				✓
LC-MS/MS Triple Quad	✓	✓	✓		
LC-MS (Q-TOF) High Resolution	✓	✓			
Automated Sample Prep	✓				
GF-AA		✓	✓	✓	
ICP-MS		✓	✓	✓	
XRD					✓
EDXRF				✓	

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SHIMADZU

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