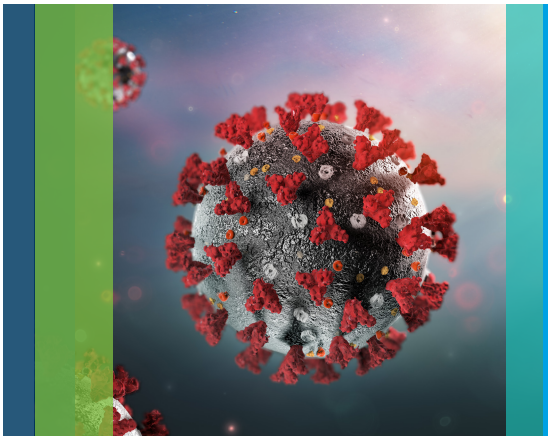

The Agilent Cary 630 FTIR Spectrometer

Applications in infectious diseases research

Agilent's mission is to "advance the quality of life". Infectious diseases affect the lives of millions all over the globe as new pathogens emerge and known ones evolve. This flyer highlights specific examples of infectious disease research and where the Agilent Cary 630 FTIR spectrometer has helped advance research and discovery. We also show the benefits of the Cary 630 FTIR spectrometer for these types of analysis.

Fourier transform infrared (FTIR) spectroscopy is a key analytical tool in infectious disease research for many reasons such as:

- FTIR spectroscopy provides quantitative as well as qualitative information.
- FTIR spectroscopy can be used to measure the four most relevant biomolecule classes (lipids, proteins, carbohydrates, and nucleic acids).
- FTIR spectroscopy is a fast and easy-to-use analytical technique that provides results in seconds.
- Small-volume samples can be used with minimal or no sample preparation and generally no consumables.
- Different types of samples can be analyzed, including liquids, solids, powders, semisolids, gases, and pastes.

For more information, visit:

www.agilent.com/chem/cary630

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Trusted Answers

The Cary 630 FTIR spectrometer has been designed for today's laboratory needs using innovative technology. As the world's smallest benchtop FTIR spectrometer, the Cary 630 FTIR combines robustness, flexibility, and high performance in an ultracompact design. In a dynamic research environment, sampling needs and analytical tasks can shift quickly. As a modular system with a wide range of sampling modules, the Cary 630 FTIR can be reconfigured in seconds to be ready for any analytical challenge.

The Agilent Cary 630 FTIR spectrometer is an ultracompact, intuitive-to-use, and high performing benchtop FTIR system. The uniquely versatile modular concept allows the Cary 630 FTIR instrument to be reconfigured with precisely optimized sample modules within seconds.

In a multiuser setting, a robust and reliable FTIR instrument is key to preventing downtime and reducing the risk of compromised data. A walkup system that is easy to learn and that requires minimal training is a must.

The field-proven, robust optomechanical system of the Cary 630 FTIR features outstanding performance and reproducibility, even in humid and tropical environments. The intuitive and easy-to-use Agilent MicroLab software uses step-by-step guidance with instructive pictures to allow easy navigation through the entire analytical workflow. In addition, Agilent offers MicroLab Expert, an advanced FTIR spectroscopy software that provides a new level of analytical flexibility and spectral visualization.

The intuitive Agilent MicroLab software workflow makes finding answers with the Agilent Cary 630 FTIR spectrometer incredibly simple and reduces training needs and the risk of user mistakes.

Applications of FTIR spectroscopy in infectious diseases research include:

- Characterization of novel chemical compounds, including substance identification
- Monitoring of processes and reactions
- Binding studies
- Protein secondary structure analysis
- Antibody quantification
- Sample classification
- Identification and detection of infectious agents or biomarkers

Examples where the Cary 630 FTIR advanced infectious disease research and the investigation of biological samples are given below:

Ultrarapid Onsite Detection of SARS-CoV-2 Infection Using Simple ATR-FTIR Spectroscopy and an Analysis Algorithm: High Sensitivity and Specificity

This study used the Cary 630 FTIR spectrometer to run ATR-FTIR analysis on saliva samples that had been spiked with COVID-19 virus particles. Each sample was analyzed simply by placing a saliva swab directly onto the ATR crystal, with no need for any sample preparation or pretreatment. The subsequent IR spectra were found to have spectral peaks that could be associated with RNA. Discrimination between infected and uninfected saliva samples was achieved through machine learning based on the unique spectral information obtained using the Cary 630 FTIR.

Barauna. V. G. *et al. Anal. Chem*. **2021**, *93(5)*, 2950–2958.

Swabs of saliva were placed directly onto the attenuated total reflectance (ATR) crystal of the Agilent Cary 630 FTIR spectrometer to determine the presence of COVID-19 virus RNA.

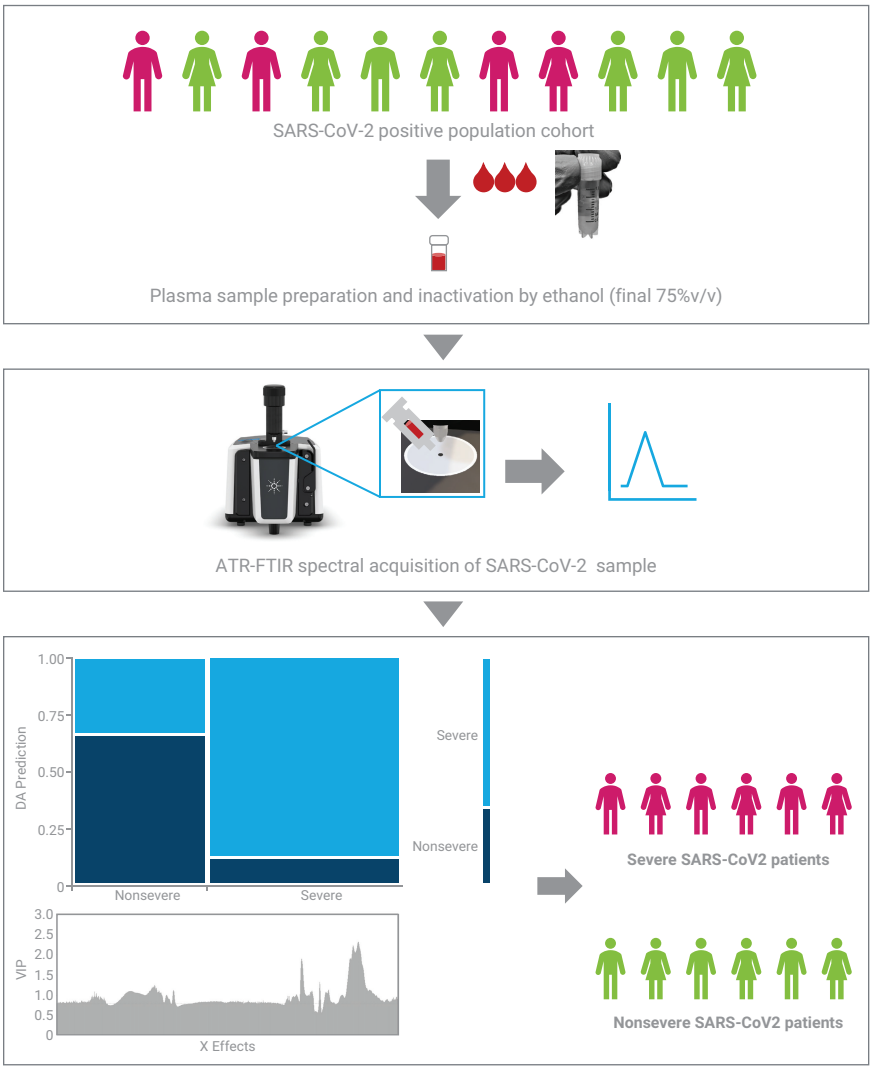
Benefits of biological sample analysis with the Cary 630 FTIR:

- No need for sample preparation
- No need for sample pretreatment
- Fast and onsite
- High sensitivity
- High specificity with machine learning

Rapid Classification of COVID-19 Severity by ATR-FTIR Spectroscopy of Plasma Samples

A rapid technique to assess the severity of the COVID-19 disease in plasma samples was developed by analyzing the samples using FTIR spectroscopy. Each plasma sample was treated simply with ethanol before a small volume was placed directly onto the surface of the ATR crystal coupled to the Cary 630 FTIR spectrometer. By studying multiple samples and analyzing key markers in the IR spectrum, a machine learning algorithm was developed to assess the severity of the COVID-19 disease in each patient. This fast and simple technique has been proposed for use in overwhelmed hospital triage settings to assess the level of care that should be assigned to each patient suffering from COVID-19.

Banerjee A. *et al. Anal. Chem.* **2021**, *93(30)*, 10391–10396.

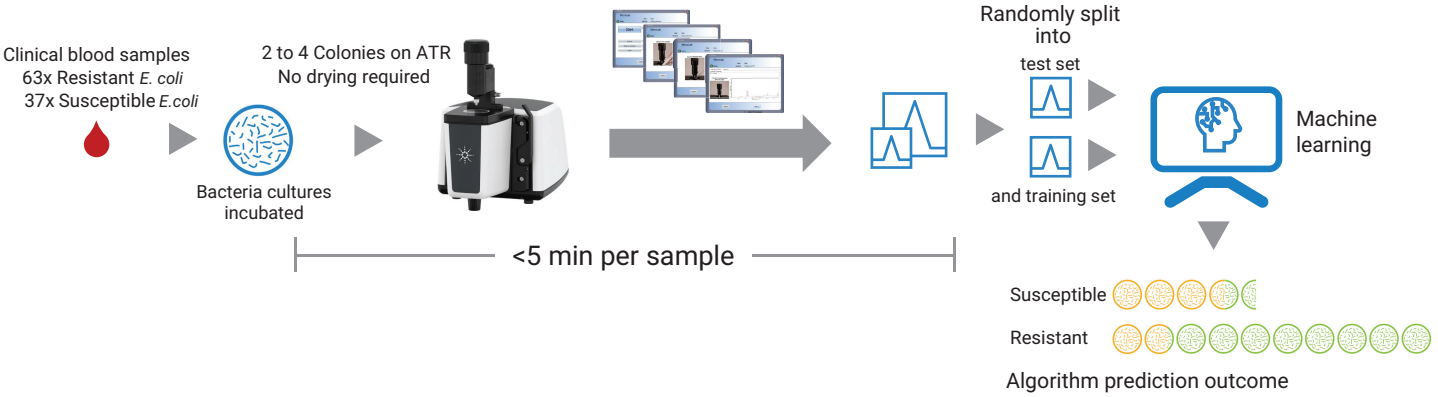


The severity of COVID-19 was assessed through this simple workflow, where plasma samples can be analyzed using ATR-FTIR spectroscopy with the Agilent Cary 630 FTIR spectrometer.

Detecting Antimicrobial Resistance in *Escherichia coli* Using Benchtop Attenuated Total Reflectance-Fourier Transform Infrared Spectroscopy and Machine Learning

A label-free diagnostic tool for determining the degree of drug resistance between different bacterial species was explored using FTIR spectroscopy. The Cary 630 FTIR spectrometer equipped with an ATR accessory was used to study multiple strains of *E. coli* by placing a sample of bacteria directly onto the ATR crystal surface, with no need for extensive sample preparation or pretreatment. A machine learning algorithm was then developed by analyzing the IR spectrum unique to each strain to determine which strains displayed drug resistance.

Wijesinghe, H. G. S. ***et al***. *Analyst*, **2021**, *146*, 6211–6219.



Samples of bacteria were analyzed for strains that display drug resistance following this simple workflow with the Agilent Cary 630 FTIR spectrometer. Bacterial samples were placed directly onto the ATR without the need for drying. The time for sampling and spectrum collection was under 5 minutes per sample, which is significantly shorter than the time needed for genome sequencing using the current gold-standard technology.

Synthesis, Characterization, ADMET Prediction, and Molecular Docking Studies Against COVID-19 Proteins of Novel 2-(3-(4-substituted aryl)guanidine-1-yl)-4-phenyl-6-(thiophene-2-yl)pyrimidines

A new variety of guanidinopyrimidine molecule was synthesized and characterized to assess new compounds that could be used to bind to the RNA proteins that are characteristic of the COVID-19 virus. Molecules that can bind to COVID-19 could eventually be used in therapeutic agents to treat or subdue the SARS-CoV-2 infection that can result from exposure to the COVID-19 virus. The molecule synthesized in this study was characterized using the Cary 630 spectrometer using FTIR-ATR analysis. The resulting IR spectrum helped to monitor the synthesis of the new compound, as well as to confirm its final structure.

Arikrishnan, J. *et al. Eur. J. Mol. Clin. Med.* **2020**, *7(3)*, 3930–3948.

The Agilent MicroLab Expert software provides advanced user spectral processing and visualization tools that help characterize newly synthesized compounds. The software identifies the best matching functional groups that might be present in the spectrum. Additional functional groups can be added from the "Matching Functional Groups" table. Color-coding indicates if the sample bands meet the interpretation criteria for the selected functional groups.

www.agilent.com/chem/cary630

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