Applications of Raman Spectroscopy in Science

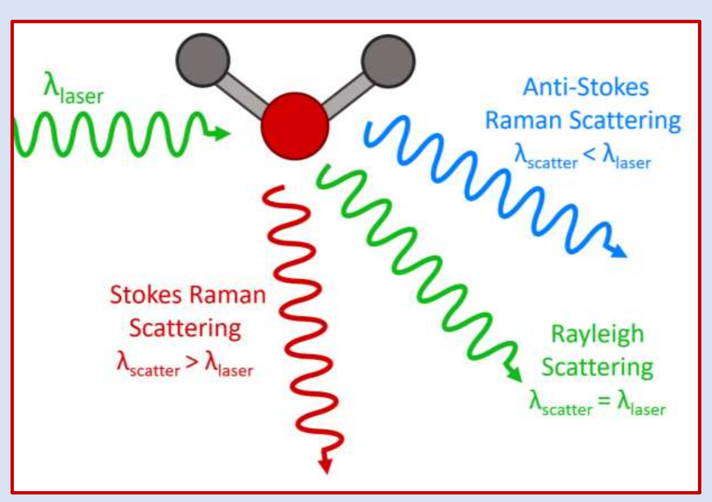
Lawrence M. Tucker, Lucas J. Scalcione, Maria Hepel
Department of Chemistry, State University of New York, Potsdam, NY 13676

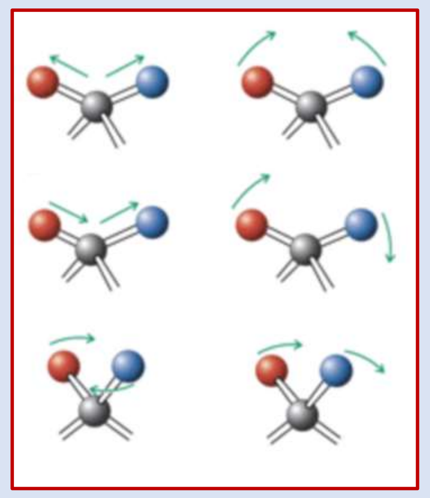
Introduction to Raman Spectroscopy

Raman spectroscopy is based on measurements of the inelastic scattering of monochromatic light from molecules. During the scattering process, the interactions of incident photons with bonding electrons of the analyte result in different, up or down, energy changes of photons, due to the exchange of energy with molecular vibrational modes.

The light scattering spectrum represents the observed intensities of these interactions versus changed energy, represented by the light frequency. Hence, the Raman spectrum is a "fingerprint" of intramolecular vibrations whose frequency is specific for the functional groups and bonds in the molecule and thus provides the means for their identification. Therefore, Raman spectroscopy can be utilized for the identification of molecules and determination of their concentration.

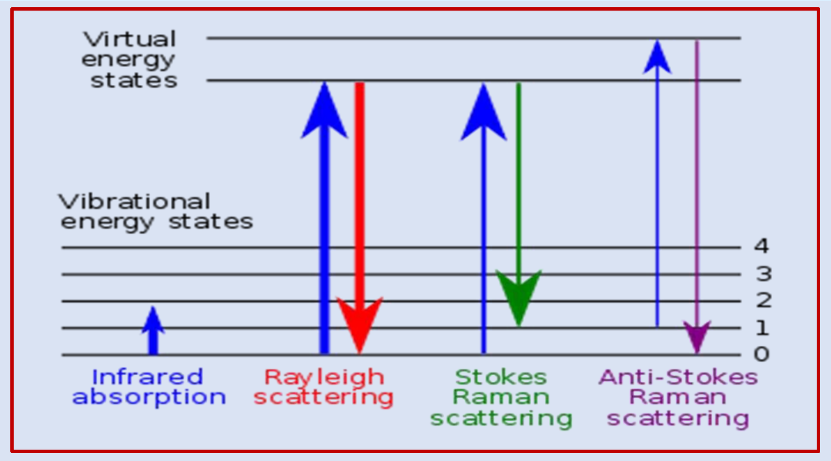
Raman scattering method is unique due to its ability to detect specific molecular vibrations with very high sensitivity, approaching 1 fM ($1x10^{-15}$ mole/L) when used in Surface-Enhanced Raman Scattering (SERS) mode.





How does Raman Work?

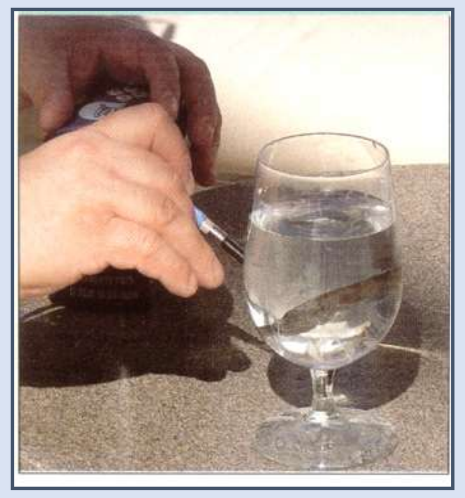
Raman spectrometers utilize the Raman effect, in which the intramolecular vibration modes of the analyte absorb photons from the incident laser beam, followed by the re-emission of photons in all directions with a de-creased energy, leading to the so-called Stockes scatter-ing. The anti-Stokes scattering is also possible, when the re-emitted photons gain the energy from the excited vibration states. Since at the room temperature, most of the molecules are at the lowest energy level, stronger Raman signals are detected for the Stokes scattering. The Raman spectrum of the scattered light provides information on the molecular structure of the analyte.



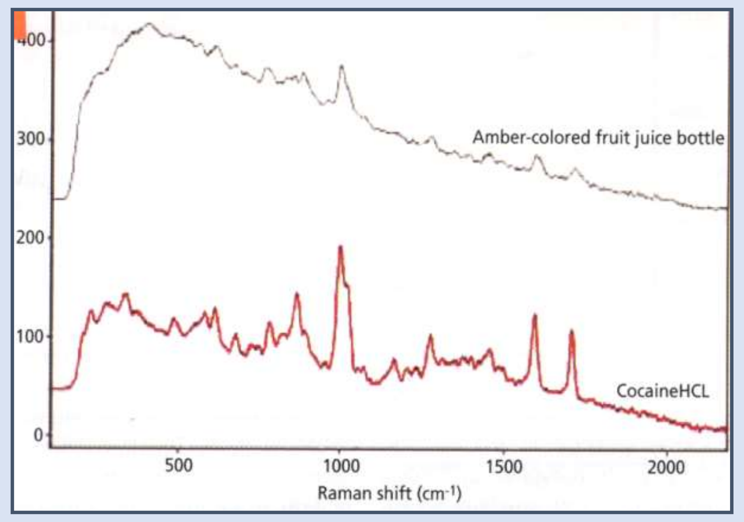
Applications

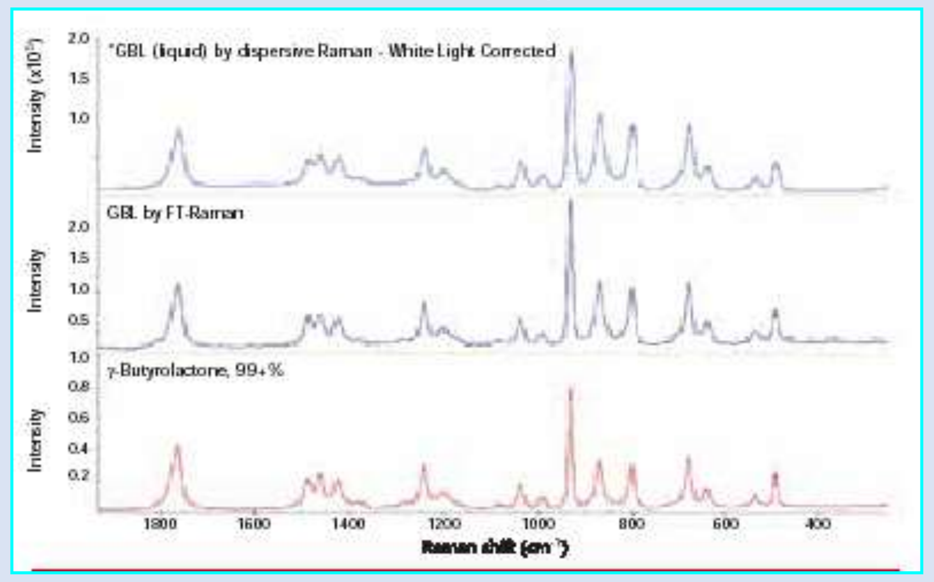
Forensic Investigations

This method can be used to detect illegal substances, explosives, counterfeit bills, diamond or glass jewelry, and even forgery.

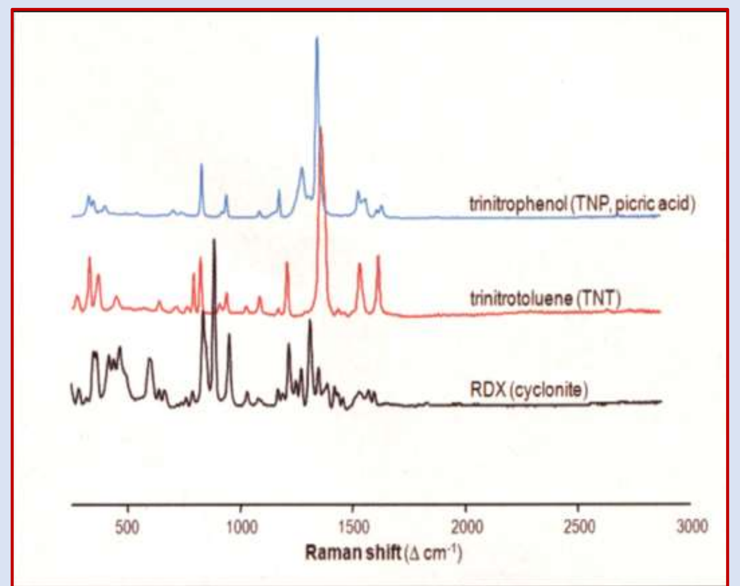


Portable drug testing allows better protection of individuals and easier evidence gathering by forensic investigators The spectra can be taken through a glass container, which does not absorb laser light, simplifying the analysis.



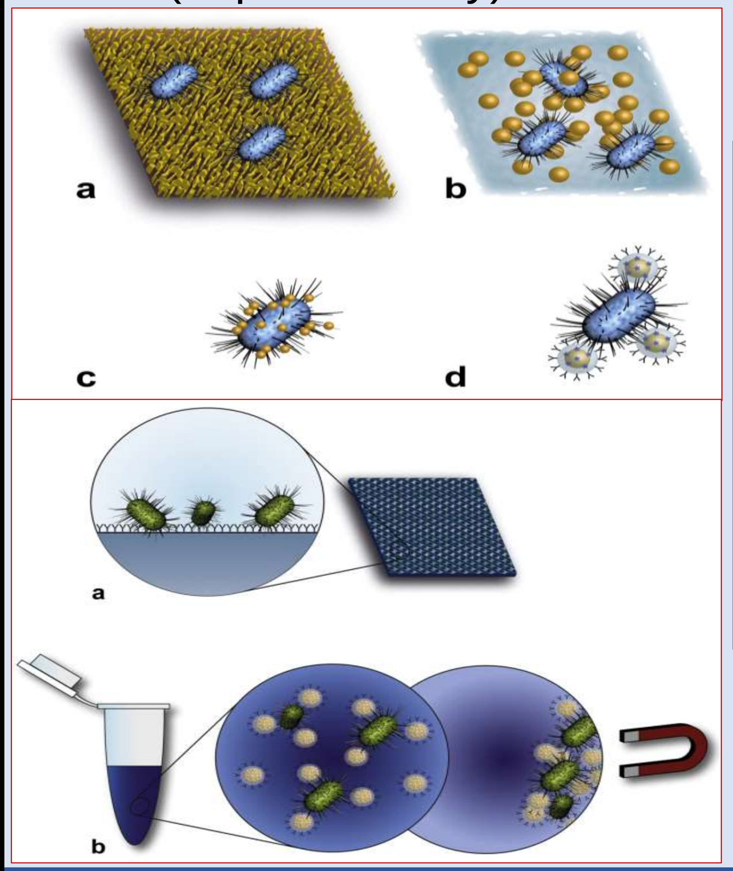


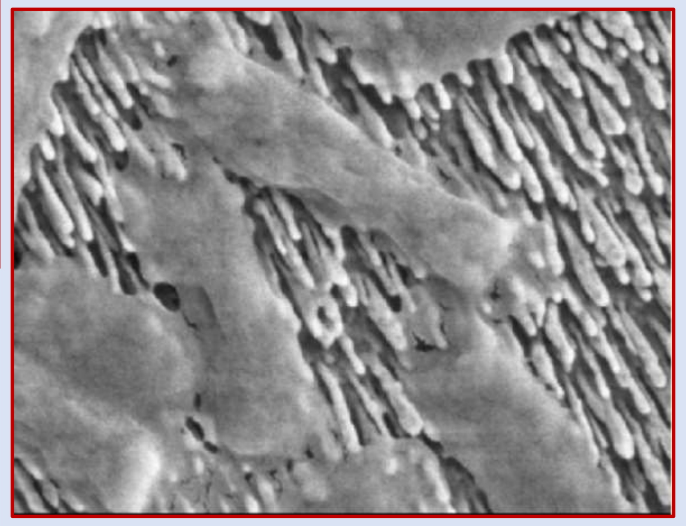
γ-butyrolactone (GBL), a precursor to GBH (Liquid Ecstasy)



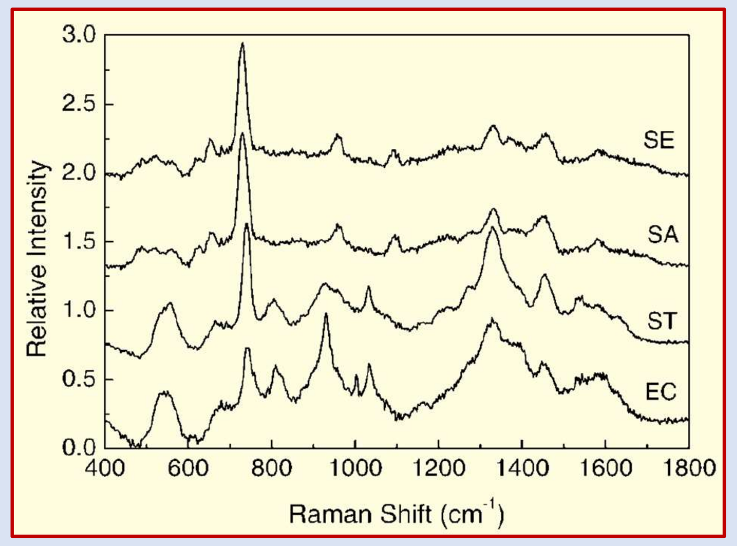
Raman spectroscopy can be employed to detect highly energe-tic materials. These materials store large amounts of energy that can be released under specific conditions, for instance in applications as explosives, propellants and pyrotechnics. The most widely applied energetic materials are neutral com-pounds: 2,4,6-trinitrotoluene (TNT), 2,4,6-trinitrophenol (TNP), 1,3,5-trinitro-1,3,5-triazacyclohexane (RDX).

Bacteria Identification





SEM image of E. coli bacteria on a silver nanorod array SERS substrate. Since the cells are not lysed, the shifts in SERS spectra are a product of cell wall biochemistry [1].

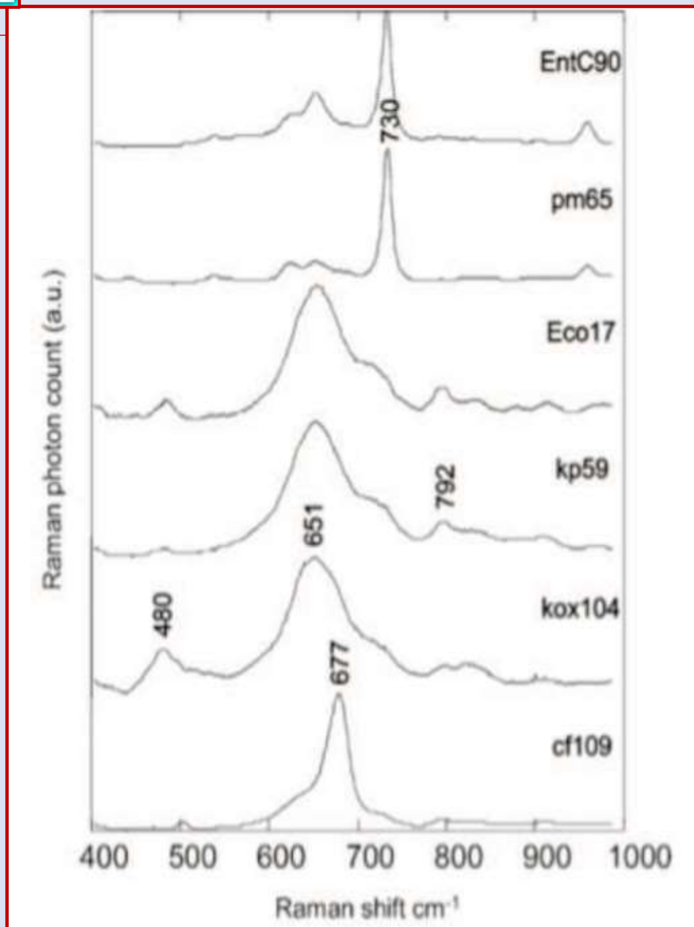


Averaged SERS spectra of four bacterial species obtained on AgNR array substrates: (EC) E. coli O157:H7; (ST) Salmonella. typhimurium; (SA) Staphylococcus aureus, and (SE) Staphylococcus epidermidis (from Ref. [1]).

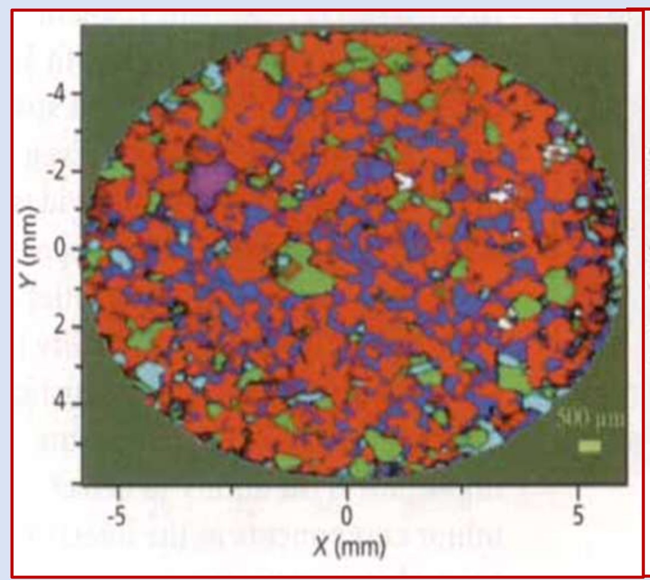
Raman light scattering is not limited to just molecules, it can also be used to detect specific micro-organisms with unique Raman shift 'fingerprints'.

Bacteria that have been coated with, attached to, or surrounded by conductive nanoparticles made of gold or silver can be detected using Surface-Enhanced Raman Spectroscopy (SERS). Once immobilized and separated, the bacteria can be scanned with SERS to provide identification.

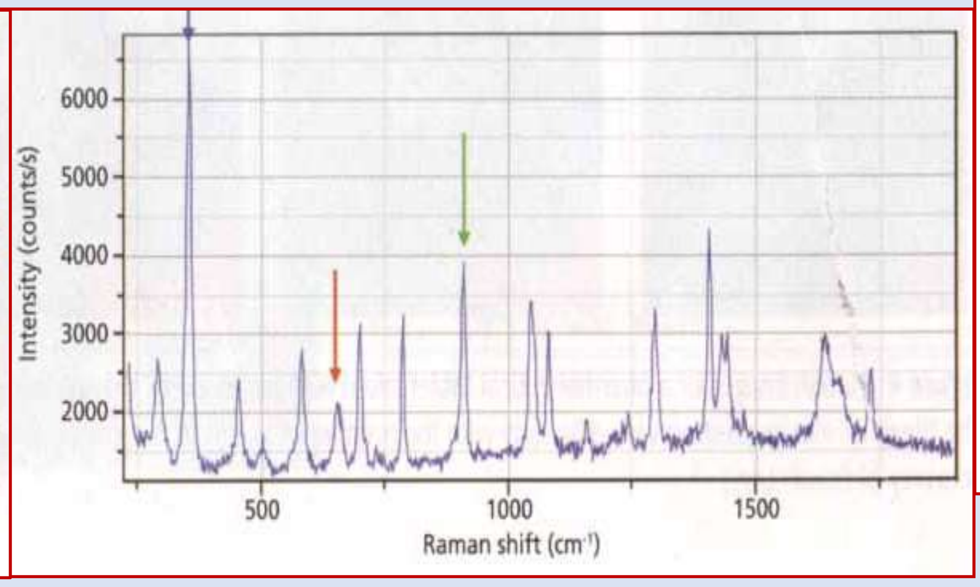
Spectra on the right: Intrinsic SERS signals [3] for urinary tract bacteria (EntC90: *Enterococcus spp.*; pm65: *Proteus mirabilis*; Eco17: *Escherichia coli*; kp59: *Klebsiella pneumo-niae*; kox108: *Klebsiella oxytoca*; cf109: *Citrobacter freundii*),



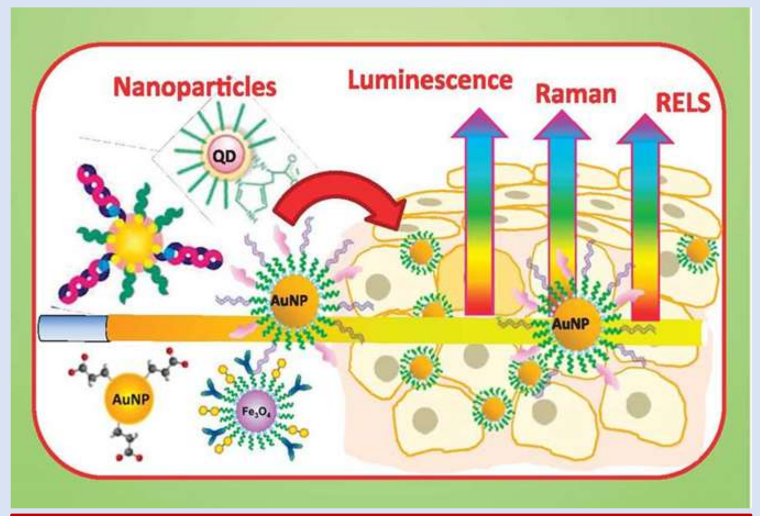
Drug Testing and Targeted Delivery



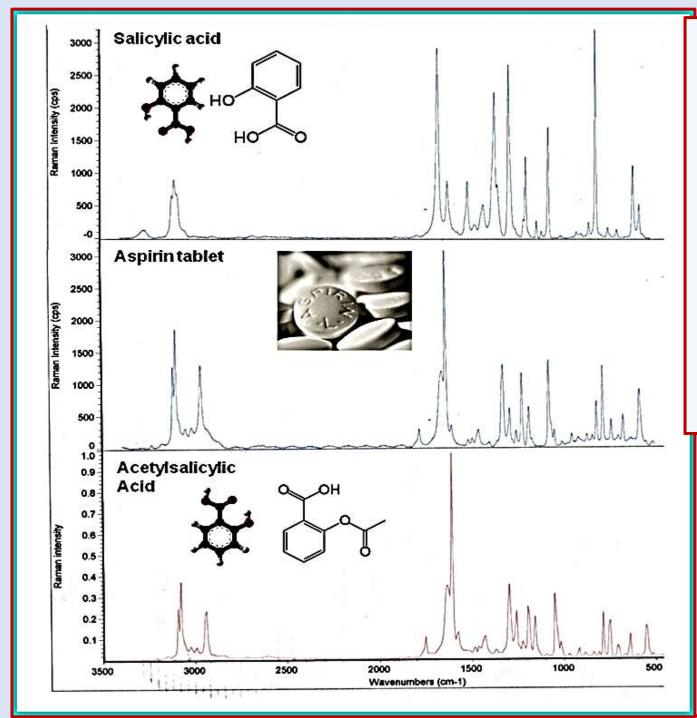
Mapping of a composite drug pellet using Raman spectroscopy.



Raman sensors and assays have been designed for testing of drugs, mapping compo-site pellets, develop-ment of nanocarrier-based drug delivery systems [5] and studies of anticancer drug interactions with DNA [6].



Raman spectroscopy has been applied in designing and testing of novel targeted drug delivery systems [5].



SERS spectra of drugs reveal the drug composition. The SERS spectra shown in these graphs were obtained for:

(a) salicylic acid,
(b) Aspirin tablet, and
(c) acetylsalicylic acid.

Conclusions

Raman spectroscopy is a rapid, highly sensitive, and effective tool for the identification of molecules and micro-organisms. Due to the widespread need for identification of materials and contaminant in industry, science, and medicine, it becomes one of the most sought after analytical techniques. Using the SERS effect, chemical com-pounds can be detected down to fM levels (1 in 10^{15} molecules).

References

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