SWOrRD

For direct detection of specific materials in a complex environment

SWOrRD

- **S**wept
  - **W**avelength
    - **O**ptical
      - **r**esonant
        - **R**aman
          - **D**etector

RAMAN EFFECT

Raman scattering or the **Raman effect** (/□rɑː mən/) is the inelastic scattering of a photon. It was discovered by Sir Chandrasekhara Venkata Raman and Kariamanickam Srinivasa Krishnan in liquids,[1] and by Grigory Landsberg and Leonid Mandelstam in crystals.[2][3]

From Wickipedia

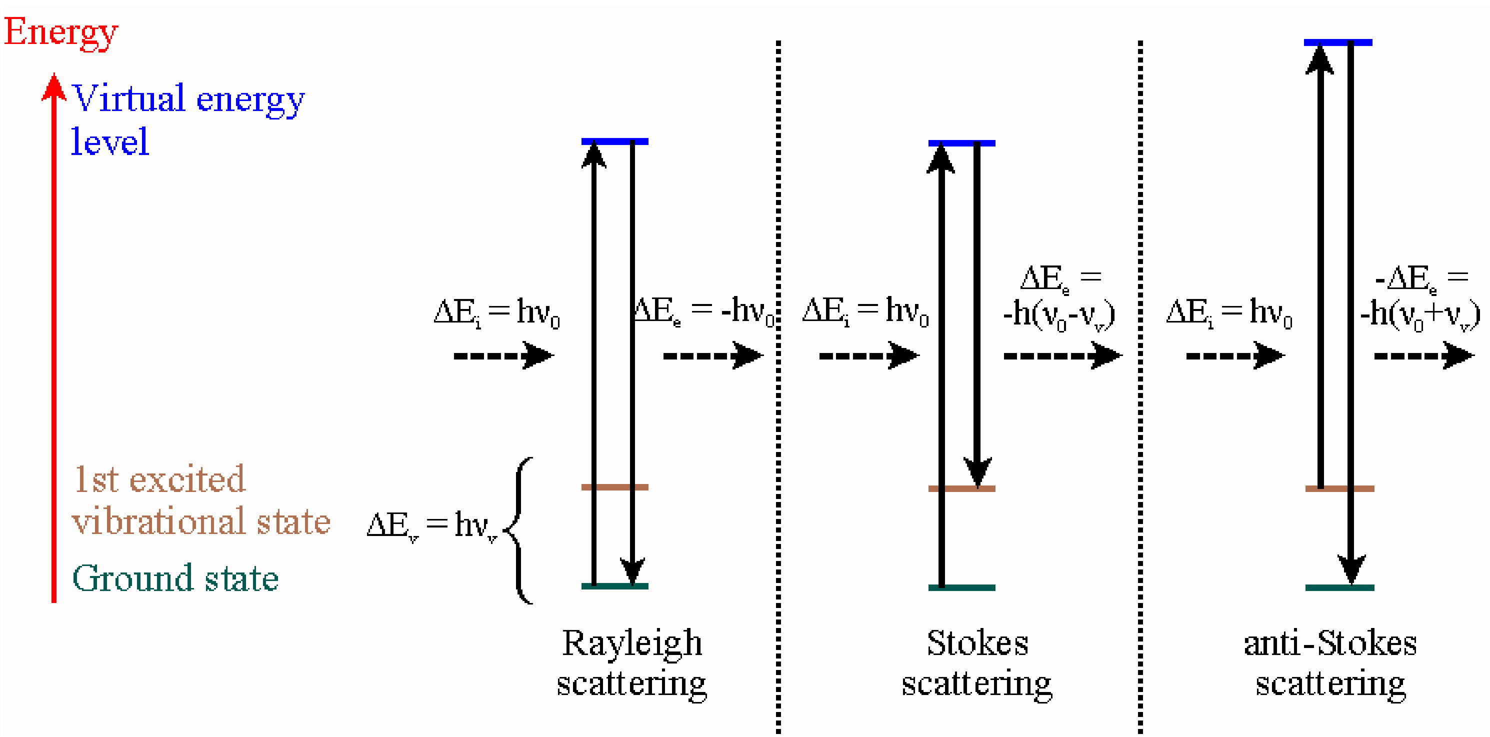
Nobel

Laureate

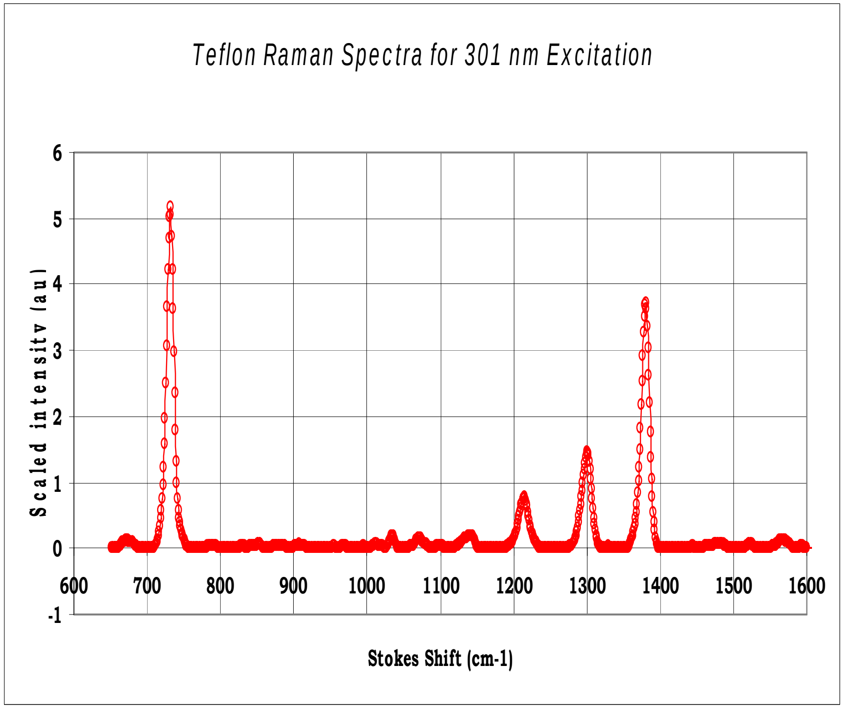
Physics

1930

Quantum “view” of Raman Scattering



- Raman scattering is **inelastic** and produces photons shifted in wavelength relative to the illuminating light.
  - **Stokes** → shifted to longer wavelengths
  - **Anti-Stokes** → shifted to shorter wavelengths
- Raman shifted photons are characteristic of the scattering material and can provide identification and information about molecular structures and bonds. **Teflon** is shown here.



W.H. Nelson, R. Manoharan, J.F. Sperry, Applied Spectroscopy Reviews 27(1) pg. 67-124 (1992).

Escherichia coli

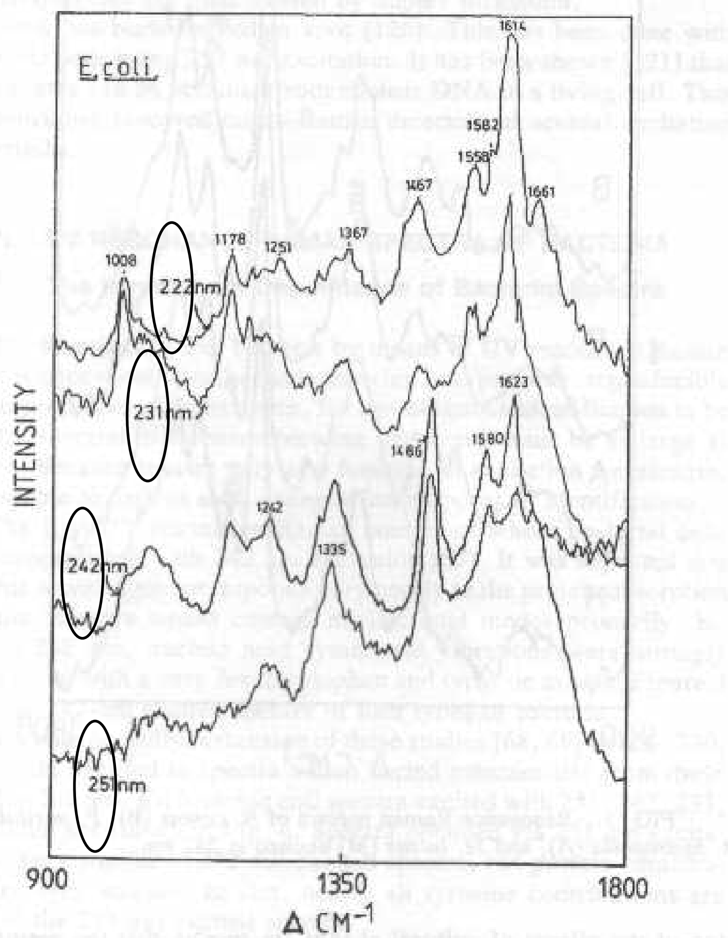


FIG. 4. **Resonance Raman spectra of *E. coli* excited at 251, 242, 231, and 222 nm.**

Frequency/wavelength effect on cross section or scattering probability

- Scattering for all components is proportional to the incident frequency to the **4th** power
  - Many formulations use the shifted frequency resulting in a correction to the stokes and anti-stokes amplitudes.
- The cross section for individual Raman lines depends on the induced polarizability (induced dipoles) for that state.
  - The cross section will be a function of **frequency/wavelength**.
  - At shorter wavelengths there may be resonance and the cross section will dramatically increase.
- Raman shifts are an absorption mechanism.

- frequency agile laser operating in the Deep Ultra-Violet (210 – 320 nm) spectral region.
  - Narrow bandwidth laser line, suitable for Raman spectra.
  - Capable of tuning to arbitrary wavelengths in 0.1 nm steps.
  - Rapid (< 1 sec) tuning between wavelengths.
- Produces 2-D Raman spectra that enhance both detection and specificity.
- Operates in other spectral regions from VIS to NIR, up to 2000 nm, as required.

The SWOrRD laser uses a gain-switched Ti:sapphire oscillator, which operates at 5 kHz and generates 18-ns pulses tunable from 700 to 940 nm in 1-nmincrements.

The laser beam is 2 mm in diameter and is well described by a TEM00 mode. Light from the oscillator is frequency converted to either third or fourth harmonics for an ultraviolet (UV) output from 210 to 280 nm, with a spectral width of 4 cm-1.

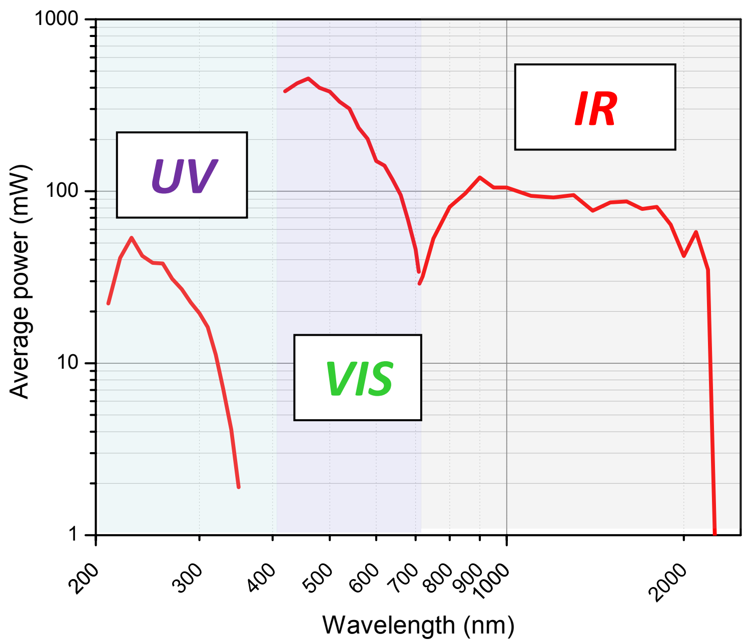
Tuning the laser to any of 200 wavelengths is computer controlled and synchronized with the angular positions of gratings in the spectrometers.

Switching wavelengths takes 1 min.

Average power in the UV varies with wavelength from a minimum of 1 mW to a maximum of 15 mW

SWOrRD Tunable Laser Source

Based on kHz Optical Parametric Oscillator (OPO) laser technology

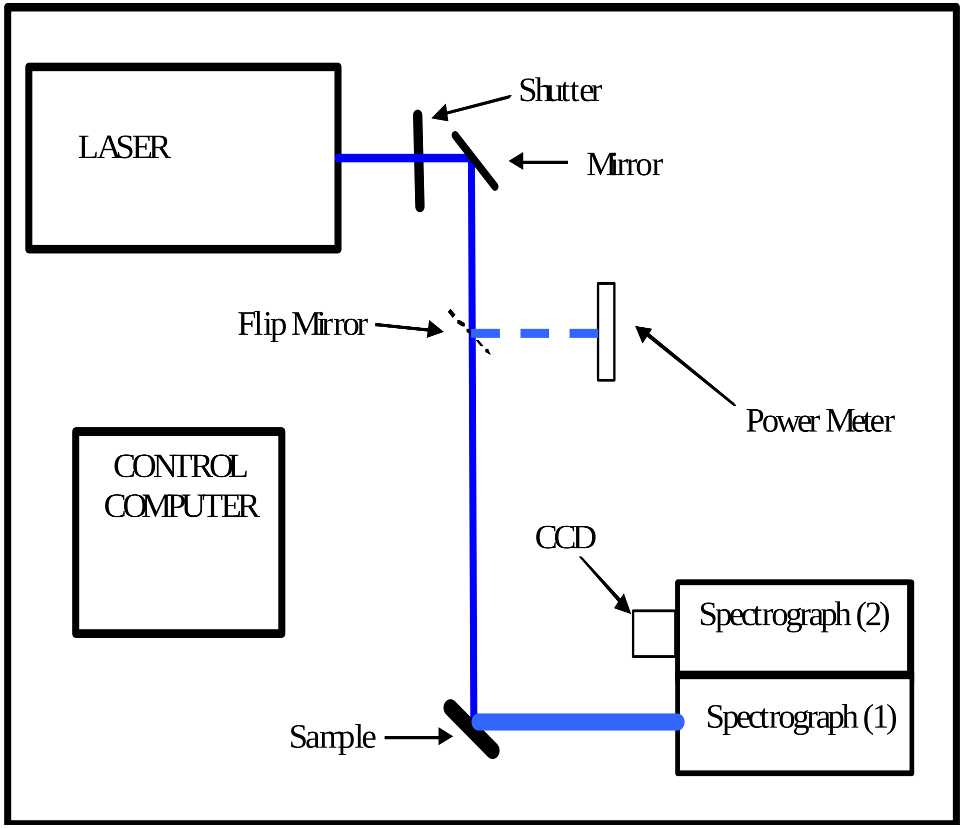


Wide Wavelength Range & High Power

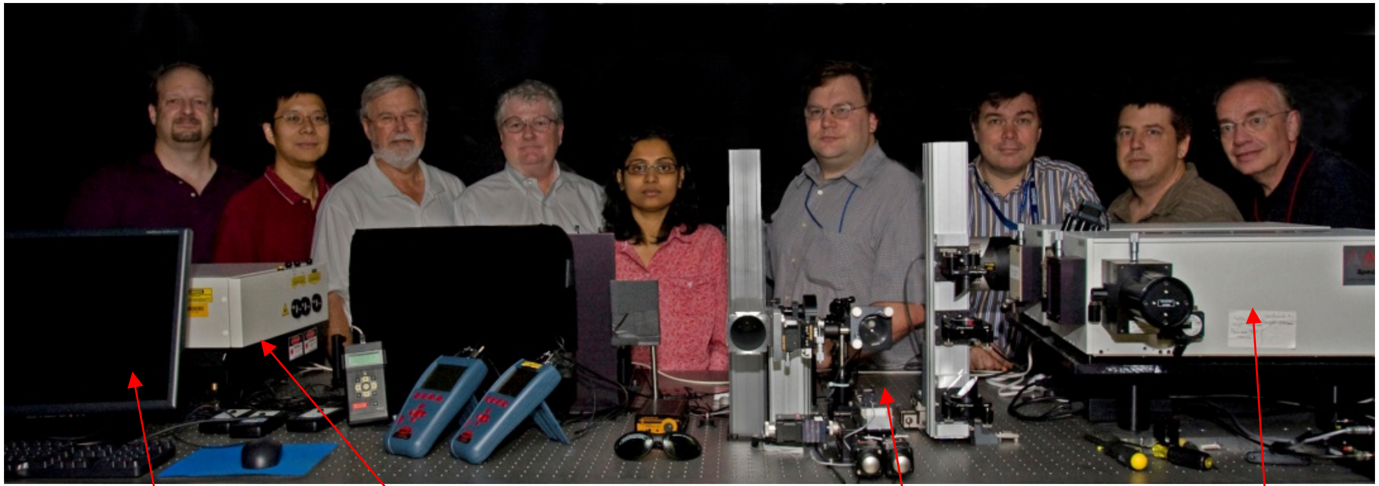
Broad tuning range
1kHz with high average power
Line width < $4cm^{-1}$
Tunable in 0.1nm steps
< 1 second to tune wavelength

SWOrRD

Block Diagram of Experiment



SWOrRD Crew

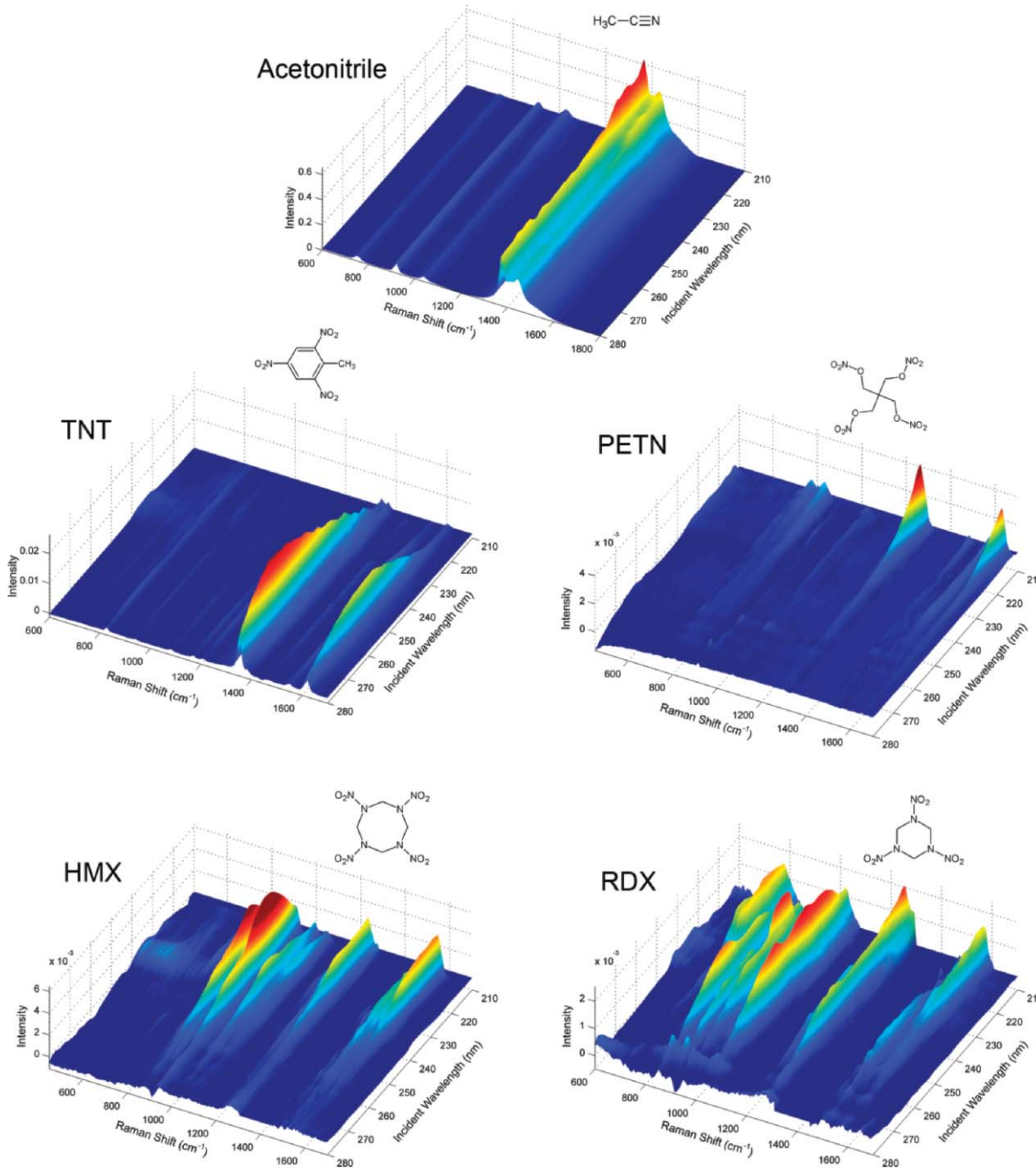


Illumination Laser

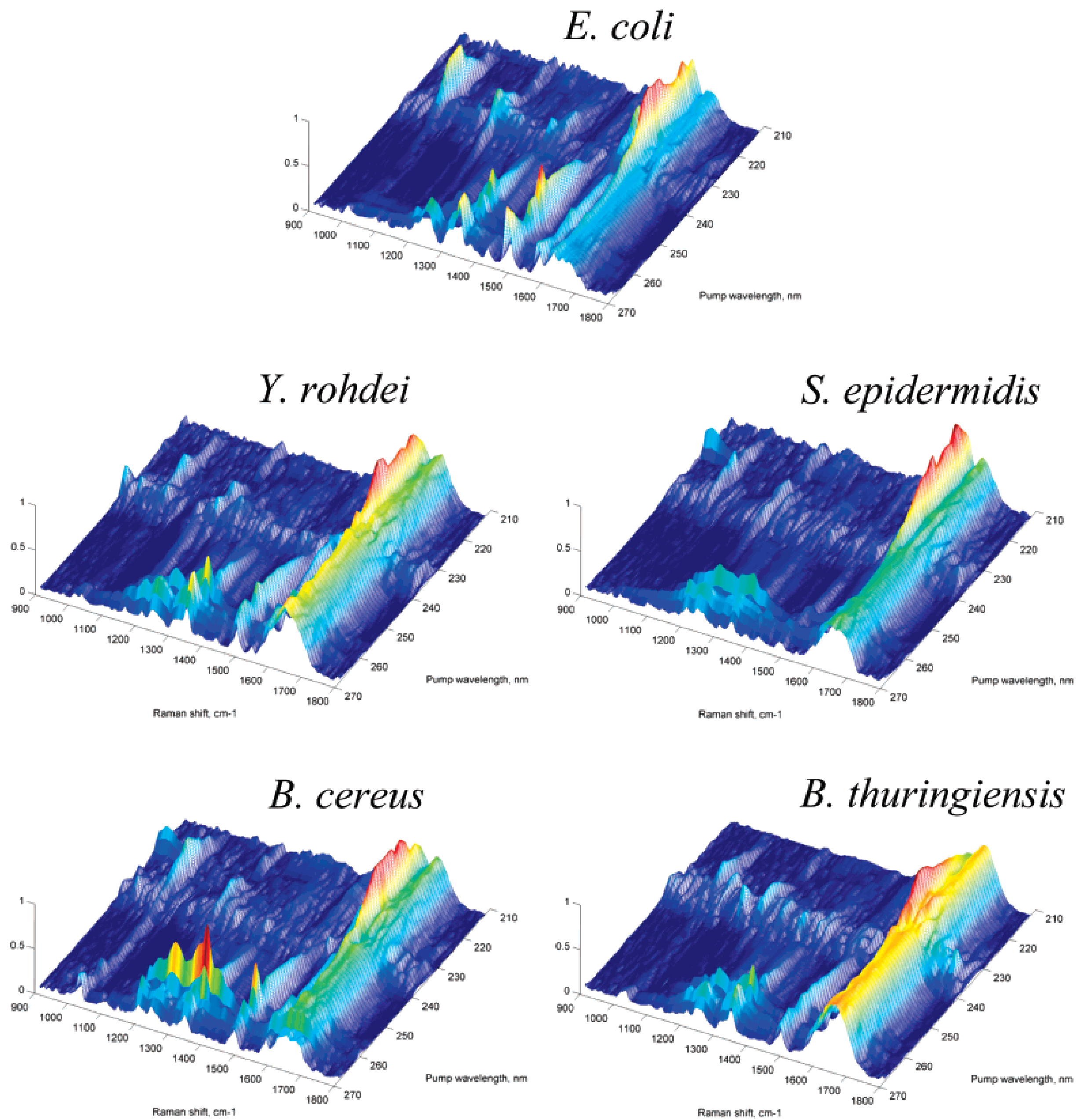
Spectrometer

Computer control

Sample holder



Acetonitrile
$H_3C-C\equiv N$
TNT
PETN
HMX
RDX
Intensity
Raman Shift (cm⁻¹)
Incident Wavelength (nm)
x 10⁻³


E. coli
Y. rohdei
S. epidermidis
B. cereus
B. thuringiensis
0
0.5
1
900
1000
1100
1200
1300
1400
1500
1600
1700
1800
Raman shift, cm-1
210
220
230
240
250
260
270
Pump wavelength, nm

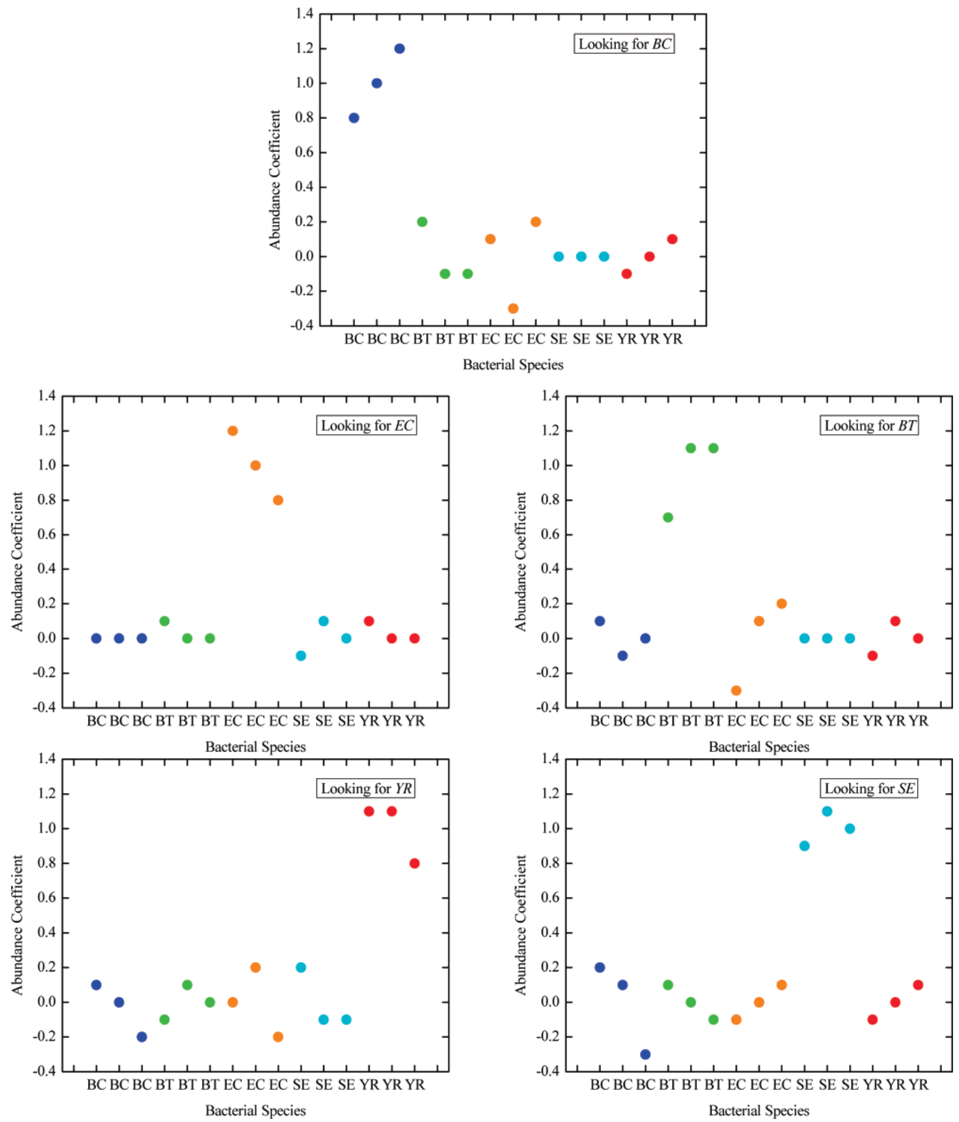


Figure 3. ORASIS identifying bacteria. Panels show the results of a search for a different bacterial species within each of 15 samples, shown on the horizontal axis. The vertical axis is the ORASIS abundance coefficient indicating the presence or absence of sought-for bacteria.

Potential Applications

(incomplete list)

- Chemicals
  - Warfare agents/Hazardous
  - Content/Composition
- Biologicals
  - Warfare agents
  - Pathogens (*in situ*?)
  - Tissue
- Pharmaceuticals
  - Identification/contamination/counterfeit
- Mineral Composition
  - Nuclear Material (Ore) point of origin
  - Paints/Inks

Improvements

(incomplete)

- Laser
  - Size/weight/efficiency
- Sample
  - Collection/preparation/handling
  - Illumination/light-collection efficiency
- Spectrometer/Detector
  - Light efficiency
  - Simplicity/size/weight
- Analysis
  - Optimization/discrimination/sensitivity

applied spectroscopy

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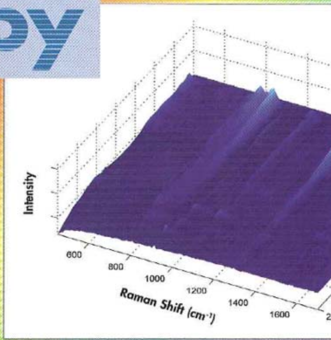
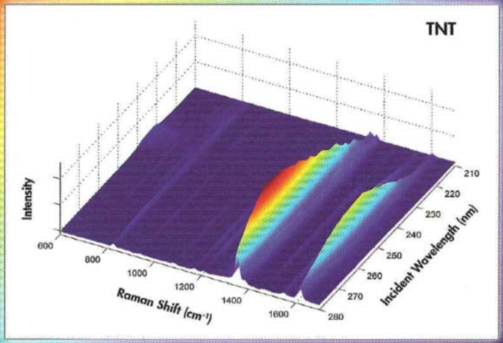
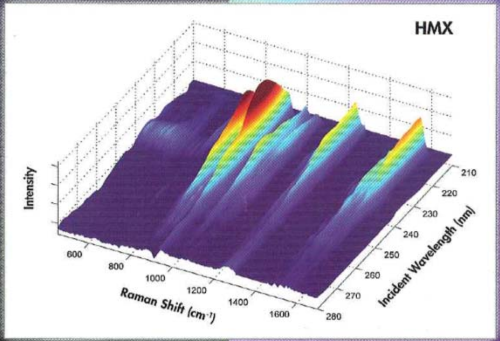
50th Anniversary
Society for Applied Spectroscopy
1958 2008

Coblentz Society Newsletter







2D UV RESONANCE RAMAN SPECTROSCOPY OF EXPLOSIVES

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