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Title:
Deep UV Raman & fluorescence spectroscopy for in situ process analysis

Authors:
William F. Hug, Q. Nguyen, M. Reid, Kripa Sijapati, & Ray D. Reid
Photon Systems, Inc., Covina, CA

Symposium:
Process Analytical

Significance:
Provides fluorescence-free Raman plus fluorescence information to identify/quantify compounds of interest in complex matrices.

Abstract:
Introduction
Raman and fluorescence spectroscopy are becoming increasingly common analytical methods for real-time, on-line and in-line, in situ monitoring of product quality in a variety of pharmaceutical, chemical, and biological manufacturing environments. The major shortcomings of Raman spectroscopy conducted in the near UV, visible, and IR are that: 1) highly efficient fluorescence emissions from targeted and surrounding materials within the excitation volume of a sample often obscure the Raman signature of the materials of interest, and 2) Raman signal strength is diminished due to Rayleigh Law and lack of resonance effects. This is especially true of simple organic compounds and biological materials such as amino acids, proteins, peptides, and whole microbial organisms as well as a wide range of pharmaceutical ingredients. In addition, the essential and informative fluorescence features of many organic and biological materials are not excited when at wavelengths longer than 260 nm.

Method
Unless excitation occurs at wavelength less than about 250 nm, there is significant overlap between Raman and native fluorescence spectral regions from a wide array of organic and biological materials including active pharmaceutical ingredients and excipients. This overlap obscures weak Raman emissions and alters the emission spectra of fluorescence emissions due to strong CH and OH Raman bands, both of which reduce the fidelity of spectral classification. This overlap is considerably worse for excitation above 260 nm.

Raman emissions provide information about the chemical bonds within the mixtures present in the excitation volume of detection. Fluorescence emissions provide complementary information about the overall electronic configuration of the targeted material. Together, Raman and fluorescence information more fully describe the chemical compounds of interest. Simultaneous acquisition of both forms of emissions coupled with chemometric analysis enables detection and characterization of a wide range of organic and biological material not possible when excitation occurs in the near UV, visible, or IR.

Results
We will describe new, compact, low cost, instrumentation employing deep UV excitation to address these growing applications.

Novelty:
Deep UV, Fluorescence free Raman, fluorescence, product quality, pharmaceutical, chemical, biological, manufacturing