Fluorescence and surface-enhanced vibrational spectroscopies of lawsone and plumbagin

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© 2016, Copyright © Taylor & Francis Group, LLC. The natural dyes lawsone and plumbagin (1,4-naphthoquinones) were studied by using fluorescence, Raman, infrared (IR), surface-enhanced Raman scattering (SERS), and surface-enhanced IR absorption. From the absorption spectrum, it was possible to infer that the enol-lawsone tautomer concentration decreases in silver colloidal solution. Plumbagin dimers, both in water and in silver colloidal solution, were identified from the fluorescence band profile and surface-SERS spectrum. The SERS spectrum of lawsone was obtained by using silver colloidal solution after 12-hour settle; the keto and enol lawsone silver colloid interaction occurs. The assignment of Raman and IR bands of both dyes was calculated with density functional theory calculations. Only a monomeric structure of lawsone interacting with a silver cluster model was predicted. The monomer adopts a nearly coplanar orientation onto the silver surface; the shortest distance is 3.2 Å, s