Our research interest is in detections of chemical and biological threat. Recent we development a study to determine the most stable conformation and orientation of L-tryptophan (L-Trp) on gold and silver nanoparticles and to investigate how these parameters were affected by analyte concentration, nanoparticle size, and pH. The purpose was to determine if L-Trp molecules interact with the nanoparticles through the carboxylate end, through the amino group end, or both. The applications of this study in biophysical and medical diagnosis are varied and could open up new opportunities in these fields. In addition, the work has the potential to enrich chemistry and nanotechnology, offering new approaches for future research. The findings represent a breakthrough in our understanding of L-Trp and nanoparticles and contribute significantly to biophysics and medical diagnostics. Surface-enhanced Raman scattering (SERS) spectra of L-Trp in the 200–3500 cm^{-1} spectral range were obtained using a 785 nm laser for excitation. Gold and silver nanoparticles were synthesized using the citrate reduction method. The experimental procedure developed included the use of electrolytes (NaCl) for colloid activation resulted in very high SERS signals. The nanoparticles surface charge was modified by changing the pH of Au and Ag colloidal suspensions in the range of 2 to 11. The obtained SERS spectra suggest that for small-size nanoparticles, high concentrations of L-Trp must be used, and for large-size nanoparticles, the opposite was needed to achieve high sensitivity of detection. The prominently enhanced intensities of stretching vibrations in the COO^{1-} group in the SERS spectra strongly suggest that the carboxylate group attaches to Ag nanoparticles. In contrast, for gold nanoparticles, a new band at ~ 2136 cm^{-1} was observed, suggesting that the amino group of L-Trp is attached to Au in its neutral form. We complement our analyses with theoretical modeling, using the Density Functional Theory (DFT) program on molecular models in which L-Trp interacted with the AgNP and AuNP substrates in neutral, cationic, and anionic forms.

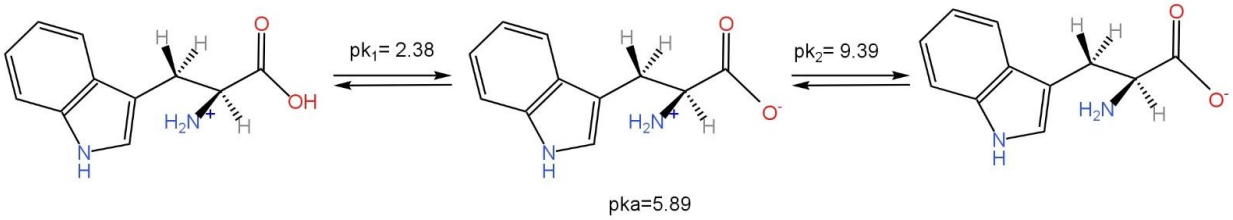

Figure 1. Three ionic molecular forms of L-Trp

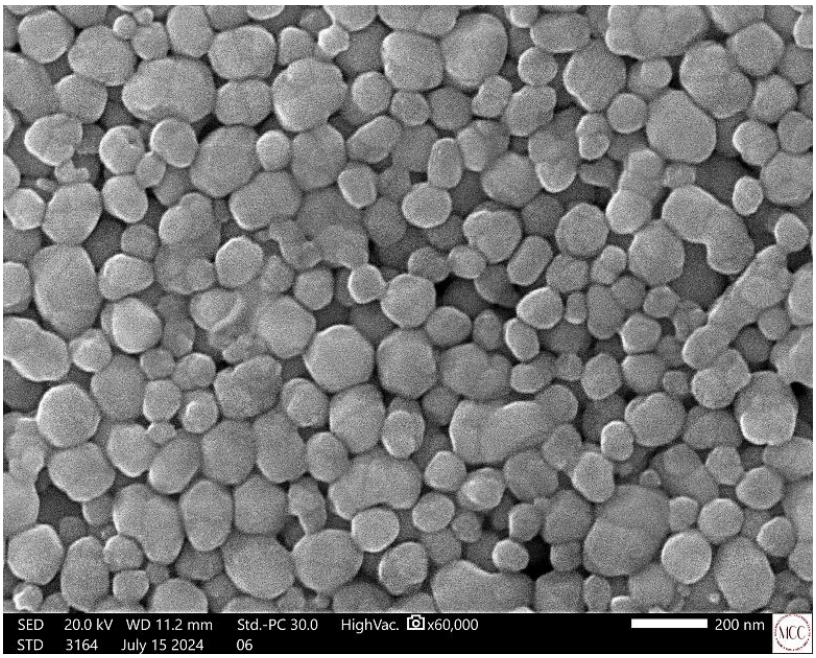

Figure 2. FE-SEM micrographs obtained for AgNPs

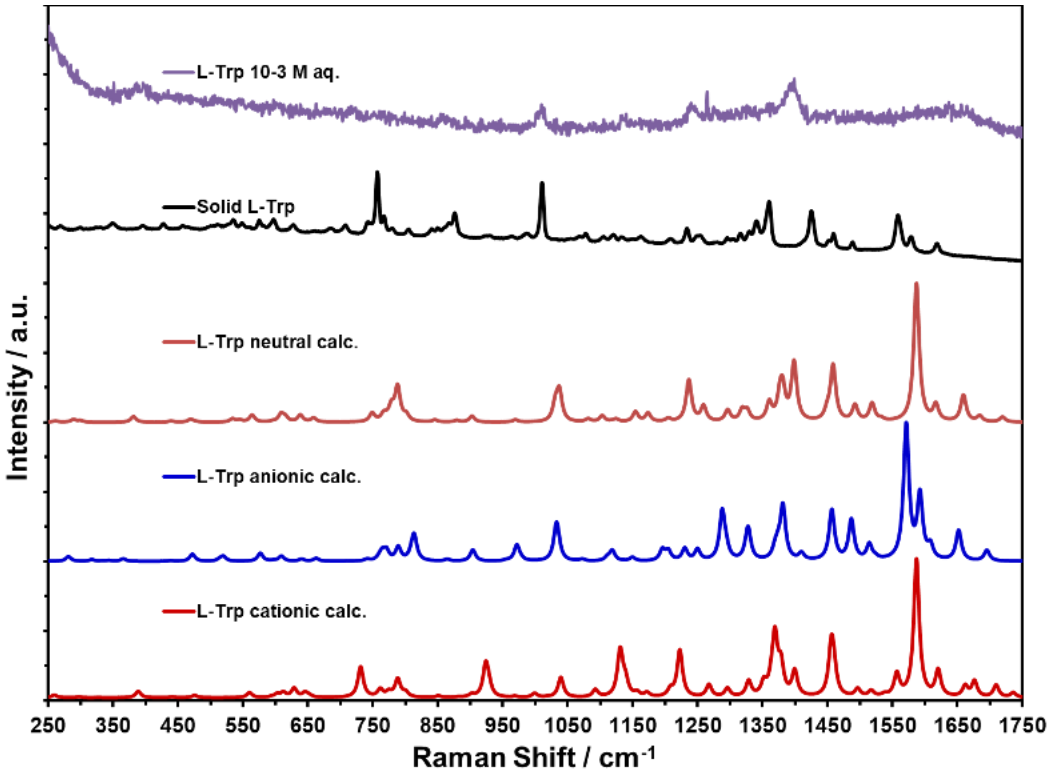

Figure 3. Comparison of Raman spectra of L-Trp experimental: (a) NR spectrum of L-Trp aqueous solution; (b) NR spectrum of solid; (c) calculated Raman spectrum zwitterion; (d) calculated Raman spectrum of anionic form; (e) calculated Raman spectrum of cationic form.

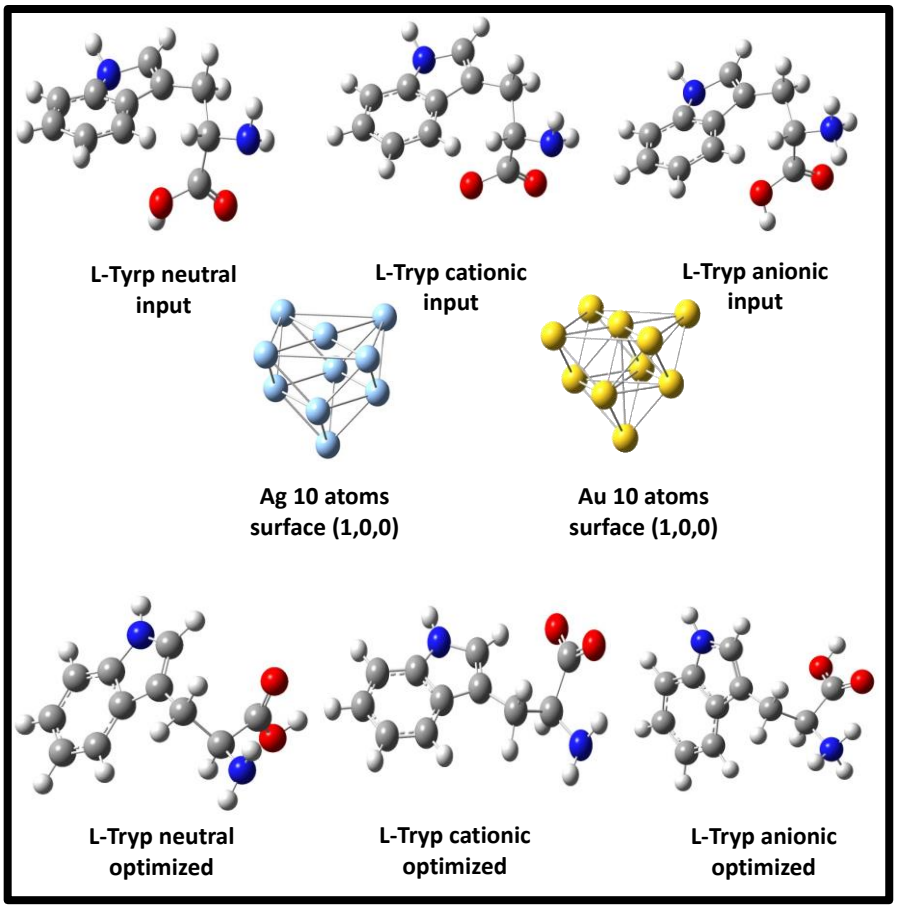

Figure 4. Optimized geometries of inputs and outputs for calculations of L-Trp with AgNP and AuNP: (a) L-Trp zwitterion, cationic and anionic form of L-Trp and 10-atom surface representations for Ag (1,0,0) and Au (1,0,0)

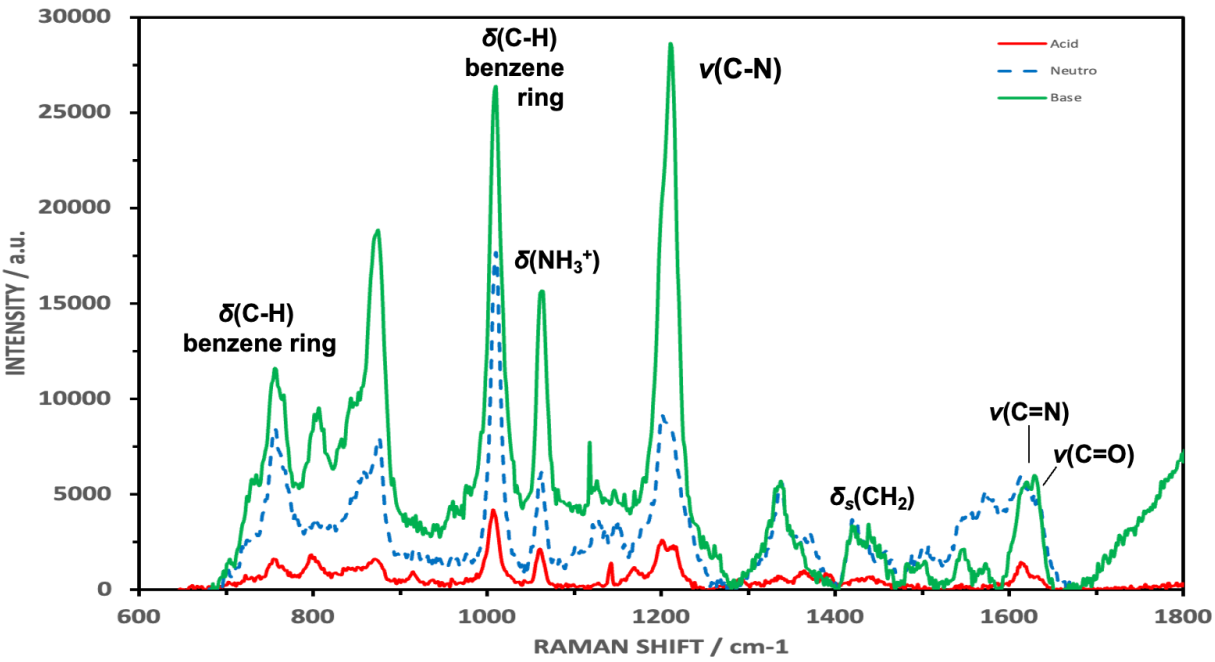

Figure 5. SERS spectra of L-Trp AuNRs/SS: (Red) pH = 5.45, (Blue) pH = 7.35, (Green) pH = 9.21.