A study of vibrational and structural properties of L,L-Dileucine hydrophobic dipeptide (molecular formula $C_{12}H_{24}N_{2}O_{3}$) is reported. The L,L-Dileucine is formed by two hydrophobic amino acids, L-Leucine, through a peptide bond. Individually this compound have many important properties, L-Leucine is important to structure and function of many proteins and enzymes. We have performed measurements of Raman and Fourier transform infrared spectroscopy, between 3500-50 cm$^{-1}$ and 3500-400 cm$^{-1}$, respectively, at ambient conditions. To support the experimental results calculations using the density functional theory (DFT) with B3LYP functional, 6-31G ++ (d, p) basis sets and the polarizable continuum model of solvation in an isolated molecule in the zwitterionic form were done. The assignment of the normal modes was described by the potential energy distribution analysis. In this way, it was possible to analyze the vibrational and structural properties of L,L-Dileucine, making an assignment of each vibrational normal mode of the molecular structure, associating with those results obtained experimentally.

References