# ABSTRACT

Carotenoids are a group of bioactive naturally occurring pigments have received much attention, because of their wide distribution, structural diversity and numerous functions. Out of these carotenoids, formation of molecular aggregates of β-carotene; extracted from *Murraya koenigii* and Lutein; extracted from *Tagetes erecta*, by means of their high and low initial concentrations and varying water /ethanol ratio were studied with the aid of spectral shift and the shape of UV-Vis absorption and fluorescence emission spectra obtained at room temperature (298 K).

The $S_0 \rightarrow S_2$ electronic transition is responsible for the strongly allowed absorption from the ground state ($S_0$) to second lowest energetic excited state ($S_2$). This transition typically corresponds to light absorption in the visible region of the electromagnetic spectrum and is the origin of the color of the carotenoids. Both neutral β-carotene and Lutein absorb maximally at three wavelengths, resulting in three-peak spectra corresponding to the 0-2, 0-1 and 0-0 transitions in the 400-500 nm region with maximum absorption ($\lambda_{max}$) at 450 nm and 445 nm respectively in EtOH. To study the complex characters of carotenoid molecules in excited state, absorption spectroscopy in not enough because $S_0 \rightarrow S_1$ ($1^1A_g \rightarrow 2\,^1A_g$) transmission is forbidden. The inherent sensitivity of fluorescence spectroscopy provides a useful alternative for probing the energies and dynamics of the $S_1$ states in carotenoids.

Formation of H-aggregates, with a blue shifted absorption with $\lambda_{max}$ around 411 nm was possible with low initial concentration of β-carotene (50 μM) and high EtOH: water (20:80) ratios. While J-aggregates, which is called red shifted, with $\lambda_{max}$ around 513 nm was formed with high initial concentration of β-carotene (100 μM) and low EtOH: water ratios. Therefore, the ability of hydrogen-bond formation is an essential factor which controls the formation of either J-aggregates or H-aggregates. Even though Lutein is dihydroxylated, it failed to form H-aggregates since the extracted Lutein was in its esterified form. However, J-aggregates with $\lambda_{max}$ around 511 nm was possible with high initial concentration of Lutein (100 μM) and low EtOH:water ratios.

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**Keywords:** *Molecular aggregates, UV-Vis absorption, fluorescence emission, J-aggregates, H-aggregates*