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Evaluation of spectroscopic, molecular modeling and UV protective cotton fabric studies over inclusion complexes of *p*-aminobenzoic acid with β-Cyclodextrin

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The inclusion complex of β-cyclodextrin (β-CD) and *p*-aminobenzoic acid (PABA) has been prepared using the co-precipitation method. β-CD and PABA ratio have been accurately weighed with 1:1 M ratio. The concentration β-CD has been varied from zero to 16×10^{-3} mol dm^{-3}. The inclusion complexation between PABA and β-CD has been monitored by using UV-Vis and fluorescence spectral analysis methods. The stoichiometry and binding constant of the PABA:β-CD inclusion complex has been determined by using Benesi-Hildebrand relation. The formation of inclusion complex is predicted by semi empirical quantum mechanical calculations and are further evaluated by using FT-IR spectral data and molecular docking analysis. In addition, ultra violet protective factor of the PABA treated cotton fabric and PABA:β-CD treated cotton fabric has been investigated. A mechanism has also been proposed for this inclusion complex.

Keywords: β-Cyclodextrin, FT-IR, *p*-Aminobenzoic acid, Inclusion complex, Cotton fabric, Benesi-Hildebrand relation