

PHYSICOCHEMICAL AND COMPUTATIONAL CHARACTERIZATION OF 2-HYDROXYETHYL METHACRYLATE WITH TOXICITY PREDICTION AND GSTP1-1 BINDING ANALYSIS

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Abstract. This study presents a computational characterization of 2-hydroxyethyl methacrylate (HEMA), a hydrophilic methacrylate monomer used in hydrogel, contact lens, and dental resin formulations. Noncovalent interaction (NCI), density overlap regions indicator (DORI), and reduced density gradient (RDG) analyses were used to examine electron density features within an isolated HEMA conformer. Molecular electrostatic potential mapping identified relatively electron rich and electron deficient regions associated with the ester and hydroxyethyl groups. Temperature dependent thermal energy, constant volume heat capacity, and entropy were calculated from 300 to 900 K within the ideal gas, rigid rotor, harmonic oscillator approximation. Physicochemical descriptors and model based ADMET and toxicity predictions were evaluated as preliminary indicators of molecular disposition and toxicity related behavior. Docking against glutathione S-transferase P1-1 produced a modest score of $-3.499 \text{ kcal mol}^{-1}$ and indicated only a possible weak association with the binding region. The docking result does not establish glutathione conjugation, catalytic turnover, or enzymatic detoxification. The findings provide molecular level information on HEMA, but they do not establish polymerization behavior, polymer scale properties, clinical biocompatibility, or safety.

Keywords: 2-hydroxyethyl methacrylate, noncovalent interactions, thermochemical properties, toxicity prediction, GSTP1-1