Biologically Inspired Material Design for Selective Removal of Estradiol Water Contaminants

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Every year, the human population discharges more than 30,000 kg of steroidal estrogens while livestock contributes close to 83,000 kg. Estradiol, a steroidal estrogen, is a prominent water contaminant in drinking water. Environmental scientists are seeking new, innovative methods of filtration in the field of water purification for estradiol eradication; however, this has not yet been developed. Estrogen, as a pollutant, may disrupt fish physiology, interrupt plant root shoot growth, and has been linked to cancer. Biologically-inspired design can potentially help scientists discover a successful filtration technique for estradiol. This study proposed the application of novel code for Protein Data Bank (PDB) mining and used visual molecular dynamics (VMD) to analyze interactions within the estradiol ligand pockets for targeted estradiol-receptive removal methods. VMD showed the presence of pi-pi T-shaped stacking and glutamic acid residue surrounding the estradiol ligand. These results suggest potential supramolecular properties and unique hydrogen bonding between glutamic acid and estradiol, which may lead to bio-inspired design of a potential sturdy estradiol-receptive removal method. The interaction distances are 3.74A° and 4.21A°, which suggests more accurate bond representations and much stronger ties among the residuals. This study demonstrates the applications of PDB mining in studying future complex protein structures and guides scientists in the precise analysis of structural data. These seminal findings can potentially help develop a novel, cost-effective, bio-mimetic filtration system using data science to mitigate and prevent the deleterious impacts of high estradiol levels.

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