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Molecular Target Homology as a Basis for Species Extrapolation to Assess the Ecological Risk of Veterinary Drugs
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Abstract:
Increased identification of veterinary pharmaceutical contaminants in aquatic environments has raised concerns regarding potential adverse effects of these chemicals on non-target organisms. The purpose of this work was to develop a method for predictive species extrapolation utilizing quantitative molecular homology based approaches for prioritizing pharmaceuticals, including veterinary drugs, based on their potential ecological risk. Because drugs are designed to target specific proteins, similarity of amino acid sequence alignments from molecular targets comparing target species to non-target species may inform predictions of species sensitivity to a pharmaceutical. This strategy was designed to take into account the quality of the alignment and to identify common conserved functional domains. A customized computer tool has been designed that automates the sequence alignments resulting in a quantitative metric that can be used to predict species sensitivity. Case examples of this approach will be presented for veterinary drugs that affect the vertebrate hypothalamic-pituitary-gonadal axis.