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Web-based Tools for Managing Aquatic Resources in Great Lakes
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Molecular Target Homology as a Basis for Species Extrapolation to Assess the Ecological Risk of Pharmaceuticals
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Abstract:
Adverse effects of many chemical contaminants, including human pharmaceuticals and other chemicals of emerging concern (CECs), are initiated through interactions with specific proteins within the cells of effected organisms. When protein targets of a given chemical are known--as is the case for many human pharmaceuticals--this information could serve as a basis for extrapolation of potential biological effects across species. Therefore, our work has focused on development of quantitative molecular homology-based approaches to predictive species extrapolation that could be used to prioritize pharmaceuticals, which are considered CECs in the Great Lakes, for potential adverse effects in aquatic organisms. Predictions about the sensitivity of the non-target species to the pharmaceutical are made based on amino acid alignment relative to the target species (e.g., humans) and associated metrics (e.g., % similarity, alignment quality, sequence integrity, and conservation of functional domains). Molecular targets and their corresponding protein accession numbers are identified using DrugBank. A computer program was developed to conduct seamless automated amino acid sequence alignments between target and non-target aquatic organisms to identify species with greater or lesser potential sensitivity to the pharmaceutical or CEC of interest.