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Pharmaceutical Concern and Prioritization Framework for Aquatic Life Effects
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Abstract:
Human pharmaceuticals and veterinary drugs are being developed and used at an increasing rate world-wide. This, and increasingly sensitive analytical techniques, have lead to recurrent detection of pharmaceuticals as environmental pollutants. The goal of the present work was to develop a scoring and ranking system (Pharmaceutical Concern and Prioritization Framework) that could be used to prioritize pharmaceuticals for ecotoxicology studies and monitoring based on known or potential adverse effects in aquatic organisms. This framework utilizes human and veterinary drug databases, containing mainly mammalian information, to gather data pertaining to individual pharmaceuticals for scoring categories predictive of effects in non-target species. The predictive categories consist of: (1) pharmaceutical absorption, distribution, metabolism and elimination (ADME); (2) drug potency; (3) pharmaceutical mode of action; and (4) species extrapolation, which considers both the primary molecular target and metabolizing enzyme(s) for the pharmaceutical. The ADME category incorporates scores for pharmaceutical LogP, molecular weight, and half life. In order to assess the pharmaceutical potency category, scores are linked to the therapeutic dose. The pharmaceutical mode of action category utilizes the "Anatomical Therapeutic Chemical" classification system established by the World Health Organization Collaborating Centre for Drug Statistics and assigns scores to each classification based on expert judgment. Species extrapolation exploits NCBI pblast to align amino acid sequences for each pharmaceutical molecular target and primary metabolizing enzyme(s) to identify homology between target vs. non-target species. The scores for this category are derived from quantitative indices of sequence homology. Finally, the framework also employs an empirical scoring category derived from reported toxicity data for non-target species, including terrestrial and aquatic organisms, where available. The scoring criteria within each category is based on parameter-specific frequency distributions determined for a subset of pharmaceuticals. The final score obtained for each pharmaceutical allows it to be ranked among other pharmaceuticals, identifying those with the greatest likelihood to produce adverse outcomes in aquatic species.