AI-Assisted Classifications of Chemicals for Systemic Toxicity

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Introduction: In the EPAA Designathon, I propose an AI-powered solution to improve systemic toxicity classification in humans, utilizing Artificial Intelligence (AI) to expedite and enhance chemical risk assessments.

Abstract: My AI-assisted approach utilizes three levels of concern to quickly and accurately assess chemical risks. By leveraging probabilistic risk assessment (PRA) and automated data analysis, I propose a new EU chemical classification system, "Chemicals 2.0," to categorize chemicals by risk level. This solution promises to reduce costs, increase efficiency, and enhance safety for both people and the environment.

Methodology:

- Component Methods: Utilizes a main prompt for AI analysis and classification of chemicals based on toxicodynamic activity and systemic availability.
- Data Integration: Combines hazard data, exposure data, and structure-activity relationship (SAR) data for weight of evidence analysis, modeling, and expert judgment.
- Criteria for Concern Levels: Severity of health effects, likelihood of exposure, and data uncertainties are considered for classifying chemicals as high, medium, or low concern.
- Scientific Basis: Integrates toxicological principles, QSARs, and machine learning for robust predictions.

Main prompt for e.g. **Google Gemini-Pro** operated by poe.com: "*What is the toxicodynamic activity and potential systemic availability of* ***common chemical name*** *or its synonyms with CAS number* ***XX-XX-X*** *and classify both as either high, medium or low for mammals?*"
Alternative prompt: "*Evaluate activity based on toxicodynamic properties and potential systemic availability based on toxicokinetic properties for* ***common chemical name*** *or its synonyms with CAS number* ***XX-XX-X*** *and classify both as either high, medium or low*"

Limitations & Future Steps:

- Data availability, chemical complexity, heterogeneity of effects, and inherent uncertainties present challenges.
- Regulatory compliance must still be adhered to.
- Future steps include validation studies, engagement with regulatory bodies, and continuous improvement as new data becomes available.
- Conclusion: The proposed AI-based solution offers a transformative approach to chemical risk assessment, streamlining classification and prioritizing safety in an innovative and effective manner.

References: Berggren E, Worth AP. "Towards a future regulatory framework for chemicals in the European Union - Chemicals 2.0." Regul Toxicol Pharmacol. 2023.

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