

Data and text mining

AOP-helpFinder webserver: a tool for comprehensive analysis of the literature to support adverse outcome pathways development

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Abstract

Motivation: Adverse outcome pathways (AOPs) are a conceptual framework developed to support the use of alternative toxicology approaches in the risk assessment. AOPs are structured linear organizations of existing knowledge illustrating causal pathways from the initial molecular perturbation triggered by various stressors, through key events (KEs) at different levels of biology, to the ultimate health or ecotoxicological adverse outcome.

Results: Artificial intelligence can be used to systematically explore available toxicological data that can be parsed in the scientific literature. Recently, a tool called AOP-helpFinder was developed to identify associations between stressors and KEs supporting thus documentation of AOPs. To facilitate the utilization of this advanced bioinformatics tool by the scientific and the regulatory community, a webserver was created. The proposed AOP-helpFinder webserver uses better performing version of the tool which reduces the need for manual curation of the obtained results. As an example, the server was successfully applied to explore relationships of a set of endocrine disruptors with metabolic-related events. The AOP-helpFinder webserver assists in a rapid evaluation of existing knowledge stored in the PubMed database, a global resource of scientific information, to build AOPs and Adverse Outcome Networks supporting the chemical risk assessment.

Availability and implementation: AOP-helpFinder is available at <http://aop-helpfinder.u-paris-sciences.fr/index.php>

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Supplementary information: [Supplementary data](#) are available at *Bioinformatics* online.

1 Introduction

Structured organization of toxicological and ecotoxicological data is now feasible using the adverse outcome pathways (AOP) framework (Ankley *et al.*, 2010). An AOP is defined by a linear combination of biological events, started from a molecular initiating event (MIE) triggered by stressors (pollutants, ionizing radiations, nanomaterials or climate stressors) connected through a series of key events (KEs) occurring at various levels of the biological organization, to an adverse outcome (AO). Biological events (MIE, KE and AO) are not linked to a unique AOP, but can be shared, allowing the establishment of Adverse Outcome Network (AON) that reflect better the true complexity of the biology. Combined with new approach methodologies (Parish *et al.*, 2020), AOPs and AONs are extremely

useful in establishing integrated approaches to testing and assessment (IATA) for environmental and risk assessment, and they aid to the development of novel nonanimal toxicity testing strategies (Delrue *et al.*, 2016).

With advances in technologies, huge amounts of data have become available, compiled in well-structured toxicological databases (e.g. CTD, CompTox), in AOP-oriented webservers (AOP-wiki, sAOP, AOP4EUpest) and scientific publications (Williams *et al.*, 2017). Innovative data mining tools are needed to identify sparse but complementary data such as Abstract Sifter allowing to have a view of the toxicological information landscape for a set of entities as chemicals (Baker *et al.*, 2017) or ComptoxAI (<https://comptox.ai/index.html>). Artificial intelligence (AI) technology, that uses natural language processing (NLP), is an interesting way to facilitate the

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