

55 - OpenTox: An open-source web-service platform for toxicity prediction

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The new European Union (EU) REACH chemical legislation will require over 9 million additional test animals, if no alternative methods for toxicity prediction are accepted. However, the number of test animals could be significantly reduced by utilizing existing experimental data in conjunction with (Quantitative) Structure Activity Relationship ((Q)SAR) models.

To address the challenge, the European Commission has funded the OpenTox (www.OpenTox.org) project to develop an open source web-service-based framework, that provides unified access to experimental toxicity data, in Silico models (including (Q)SAR), and validation/reporting procedures.

Now, in the final year of the initial three-year project, the current state of architecture, Open API, algorithms, ontologies, and approach to web services will be presented. Our experiences on current collaborative approaches aiming to combine OpenTox with other systems such as CERF, Bioclipse, CDK, and SYNERGY to create "super-interoperable K-infrastructure" will be discussed both in terms of conceptual promise and implementation reality.

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[Internet and Chemistry: Social Networking \(08:30 AM - 11:40 AM\)](#)

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