In silico Screening for Potential Endocrine Disruptors

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Endocrine disrupting activities of chemicals trigger adverse effects on organisms. While their effect on the development and reproduction of animals is well known, there is much less knowledge about their impact on human health. However, endocrine disrupters are suspected to be responsible for a number of diseases as testis and breast cancer, oligospermia of young men, or adiposis. Compounds with endocrine activity are labelled as substances of very high concern (SVHC) and are subject of regulations as e.g. under REACH.

However, there are so far no internationally harmonised criteria to identify endocrine active chemicals. Furthermore, the endocrine system is rather diverse. Despite of several already developed OECD tests to reveal respective activities, it is still not clear whether they comprise all (eco)toxicologically relevant pathways. Even more, these tests are rather expensive with respect to costs and duration. Consequently, the number of existing data is limited.

In silico tools are promising alternatives to avoid testing or at least to allow for the prioritisation of tests by screening larger compound lists. The German Federal Environment Agency holds a prototype of a structural alert model and corresponding software tool for this task. Based on it, the current study aims to significantly extend this model and to make it available as an automated tool in the software system ChemProp (UFZ Department of Ecological Chemistry 2014. ChemProp 6.2. http://www.ufz.de/index.php?en=6738).

The envisaged model will provide a decision tree to identify potential endocrine disruptors and their respective modes of action. The paper gives an overview of the approach and reports first results for several modes of action with respect to thyroid hormones.