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Chemical similarity: structuring risk and hazard assessment

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Citation

Wassenaar, P. N. H. (2022, April 19). *Chemical similarity: structuring risk and hazard assessment*. Retrieved from <https://hdl.handle.net/1887/3283611>

Version: Publisher's Version

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Propositions

“Chemical Similarity: Structuring Risk and Hazard Assessment”

By Pim N.H. Wassenaar

1. The chemical universe is diverse in structures, uses and effects, and cannot be evaluated and managed with a single measure (This thesis).
2. Computer models provide more robust predictions than individual experts (This thesis, chapter 3).
3. Experimental results derived according to test guidelines may not be as robust as commonly believed (This thesis, chapter 5).
4. Model applications and solutions in risk and hazard assessment should be fit for purpose, balancing simplicity and complexity (This thesis).
5. We will never be able to assess and manage all hazards and risks before any exposure and/or effects occur (This thesis, chapter 7).
6. The vast amount of (available) toxicological data should be used more systematically to improve the level of protection of human health and the environment (inspired by Pawar et al., 2019; Suter et al., 2020; and Wittwehr et al., 2020).
7. The quality of data used for data analysis and model development, strongly influences the reliability of the outcomes (inspired by Yang et al., 2018; and Moermond et al., 2017).
8. New approach methodologies need to be developed, not only for screening and prioritization applications, but also for the next steps in the risk assessment process (Kavlock et al., 2018).
9. Newly developed models need to be transparent and interpretable to guarantee community-wide trust and regulatory acceptance (inspired by Rudin, 2019).
10. The development and use of safe and sustainable (production of) chemicals is essential to strengthen the protection of human health and the environment (European Commission, 2020).
11. Mirror, mirror on the wall, does similarity say it all? No, but it is a very valuable aspect for risk and hazard assessments.