



Universiteit
Leiden
The Netherlands

Chemical similarity: structuring risk and hazard assessment

Wassenaar, P.N.H.

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

[Licence agreement concerning inclusion of doctoral thesis in the Institutional Repository of the University of Leiden](#)

Downloaded from: <https://hdl.handle.net/1887/3283611>

Note: To cite this publication please use the final published version (if applicable).

Chemical Similarity

Structuring Risk and Hazard Assessment

Pim N.H. Wassenaar

© Pim N.H. Wassenaar 2022

Chemical Similarity: Structuring Risk and Hazard Assessment

PhD thesis, Leiden University, The Netherlands

The research as described in this thesis was conducted at the Institute of Environmental Sciences (CML), Leiden University, The Netherlands.

ISBN: 978-90-5191-700-0

Cover: Pim N.H. Wassenaar

Design and layout: Pim N.H. Wassenaar

Printed by: ProefschriftMaken

Chemical Similarity

Structuring Risk and Hazard Assessment

Proefschrift

ter verkrijging van
de graad van doctor aan de Universiteit Leiden,
op gezag van rector magnificus prof.dr.ir. H. Bijl,
volgens besluit van het college voor promoties
te verdedigen op dinsdag 19 april 2022

klokke 13.45 uur

door

Pim Nicolaas Hubertus Wassenaar
geboren te Beverwijk
in 1993

Promotores:

Prof.dr.ir. W.J.G.M. Peijnenburg
Prof.dr.ing. M.G. Vijver

Promotiecommissie:

Prof.dr. A. Tukker
Prof.dr.ir. P.M. van Bodegom
Prof.dr. S. Suh
Dr. J.N. van Rijn
Prof.dr. E. Benfenati (Mario Negri Institute for Pharmacological Research)
Dr. E. Papa (University of Insubria)

Table of contents

Chapter 1	General Introduction	7
Chapter 2	Chemical Similarity to Identify Potential Substances of Very High Concern – an Effective Screening Method	29
Chapter 3	Evaluating Chemical Similarity as a Measure to Identify Potential Substances of Very High Concern	51
Chapter 4	ZZS Similarity Tool: the Online Tool for Similarity Screening to Identify Chemicals of Potential Concern	79
Chapter 5	Variability in Fish Bioconcentration Factors: Influences of Study Design and Consequences for Regulation	101
Chapter 6	Persistence, Bioaccumulation and Toxicity-Assessment of Petroleum UVCBs: a Case Study on Alkylated Three-Ring PAHs	119
Chapter 7	General Discussion	149
	References	163
	Summary	179
	Samenvatting	185
	Curriculum Vitae	191
	List of Publications	193
	Dankwoord	197

