



Proven expertise in
in silico predictions
and read-across

In Silico Toxicology and Ecotoxicology

Using New Approach Methods (NAM) for
Health Hazard Identification and
Environmental Risk Assessment

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SCC 
WE CARE FOR YOUR SUCCESS

IN SILICO MODELS

The increasing efforts to reduce *in vivo* tests for chemicals and active substances to a minimum, increase the importance of New Approach Methodologies (NAM). *In silico* analyses using advanced computational modelling are applied to predict the activity, property, toxicity and ecotoxicity of a substance based on the knowledge of its chemical structure.

Due to our long years' experience, we are well familiar with generating *in silico* data to fulfil regulatory hazard information requirements for active substances of plant protection products, biocides, pharmaceuticals, chemicals, cosmetic products and smoke flavourings as well as their metabolites and impurities. For a reliable prediction, we use multiple methodologies alongside an expert review. To obtain valid results, we consider the potential applicability of diverse models, the reliability (domain) of the models, the documentation of the model development and validation process and finally the acceptance of the models by authorities. Our *in silico* scientists are specialised in all relevant disciplines and work in large teams. Data they generate can be further processed and assessed based on the overall weight of evidence.

Application in regulatory frameworks

We provide our services for various regulatory areas supporting the application of *in silico* models, including but not limited to:

- **ICH guideline M7(R1)**
 - Assessment of potential genotoxic pharmaceutical impurities
 - Toxicity assessment of extractables and leachables
- **Regulation (EC) No 1107/2009 and Regulation (EC) No 528/2012**
 - Toxicological and ecotoxicological properties of active substances, metabolites and impurities, for plant protection products and biocidal products
- **REACH Regulation (EC) No 1907/2006**
 - Toxicological and ecotoxicological properties of chemicals (including skin sensitisation)
- **Regulation (EC) No 1223/2009**
 - Toxicological and ecotoxicological properties of cosmetic ingredients
- **Regulation (EC) No 2065/2003**
 - Assessment of potential genotoxic components in smoke flavouring primary products



OUR EXPERTISE

Our profound long-term knowledge of registration processes and associated data requirements in global key markets allows us to successfully handle all kinds of *in silico* requests.

The assessment generally includes:

- Generation of robust *in silico* predictions to support chemical(s) in a weight of evidence approach for internal and regulatory purposes
- Chemical category formation, grouping and selection of suitable analogues and data-gap filling (e.g. read-across)

Our scientists work with numerous *in silico* models, including:

- VEGA
- Toxtree
- US EPA T.E.S.T.
- Danish (Q)SAR Models
- Endocrine Disruptome
- US EPA EPI Suite
- ECOSAR Predictive Model
- OECD QSAR Toolbox
- Derek Nexus
- Leadscope



Please visit our website:

<https://www.scc-gmbh.de/scientific-regulatory-services/in-silico>

or contact our *in silico* experts:

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OUR SERVICES

Our team offers a full range of services to generate and interpret *in silico* data.

Following detailed analyses of the data and situation, we work out individual solutions covering regulatory requirements and meeting your specific needs. Our services include:

- Data gap analysis tailored to the specific use case
- Feasible assessments, also for structures that e.g. cannot be easily synthesised
- Applying a suite of well-validated *in silico* expert rule-based and statistical-based software tools selected in agreement with the official guidelines considering applicability and reliability (domain)
- Robust (Q)SAR analyses for different endpoints such as toxicity, ecotoxicity predictions (e.g. genotoxicity and/or endocrine disruption)
- Evaluation with expert knowledge in a weight of evidence approach
- Uncertainty analysis and optimisation of the quality of the prediction and its confidence
- Data gap filling approach, e.g. read-across including grouping of chemicals, category formation and search for suitable analogues
- Description of methods and results in state-of-the-art reports according to the respective guidance documents
- *In silico* assessments for all types of regulatory purposes
- Communication and data management, follow-up and defence of compounds including negotiations with regulatory authorities and scientific bodies

Please do not hesitate to contact us to learn how we can help you with your specific needs.

WHO WE ARE

Privately owned, independent and neutral

SCC is a privately owned, independent and neutral consulting company with an extensive global network but no commercial ties to contract research organisations. Since 1989, we have been supporting our customers with tailored solutions for their scientific and regulatory needs within and outside the EU. Our expertise extends over a broad range of areas:

- Agrochemicals & biorationals, incl. fertilisers and biostimulants
- Biocides
- Chemicals
- Medical devices
- Cosmetics and consumer products
- Pharmaceuticals
- Food contact materials
- Feed additives
- International MRL setting
- Genetically modified/edited crop (Japan)
- Legal and consortia management (SCC Legal)
- Market Analysis
- GLP-Archiving

OUR OFFICES

- **SCC headquarters, Bad Kreuznach, Germany**
- **SCC Office Berlin**
- **SCC Japan**
- **SCC UK**

All our teams in different locations consist of highly educated and team-oriented experts, mostly academics and PhDs. More than 140 professionals are employed at the headquarters in Bad Kreuznach. Our offices with their expert teams complement the headquarters and guarantee our international customers broader access to our services.

Over three decades, we have been acting on the side of our customers providing them with expert guidance and helping them to master their regulatory challenges in the EU, Asian-Pacific, Eurasian and North and South American markets.

In this time, we have established an extensive network of partners and associates in various regions to guarantee our customers access to top-qualified and first-hand expertise in their target markets. At SCC, you will find an open-minded, innovative entrepreneurial spirit backed by the expertise and commitment of a strong team. This winning combination has played a significant role in our company development. It embodies values such as high quality, flexibility, reliability and versatility, coupled with vast knowledge and a wealth of experience. And that is what drives us forward.

