

**Chris Grulke, Cheminformatician, in EPA's National Center for Computational Toxicology**

[Mailing Address](#)

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**Area of Expertise:** Dr. Grulke is an advanced cheminformatics scientist and software developer with comprehensive knowledge in integrating chemical and biological data into models for decision support. He has ten years of hands-on experience storing, integrating, visualizing and analyzing complex datasets. He also has a broad array of interests and skills including cheminformatics, toxicological modeling, exposure modeling, PBPK modeling, ADME property prediction, statistical analysis, machine learning, text-mining, natural language processing, programming, and software engineering.

**Select Publications:**

Brown K, Phillips M, Grulke C, Yoon M, Young B, McDougall R, Leonard J, Lu J, Lefew W, Tan YM. [Reconstructing exposures from biomarkers using exposure-pharmacokinetic modeling—A case study with carbaryl](#), Reg. Tox. & Pharm. 2015 73(3):689-698

Phillips MB, Leonard JA, Grulke CM, Chang DT, Edwards SW, Brooks R, Goldsmith MR, El-Masri H, Tan YM. [A Workflow to Investigate Exposure and Pharmacokinetic Influences on High-Throughput in Vitro Chemical Screening Based on Adverse Outcome Pathways](#), Env. Health Pers. 2015 <http://dx.doi.org/10.1289/ehp.1409450>. [Exit](#)

Isaacs K, Glen W, Egeghy P, Goldsmith MR, Luther S, Vallero D, Brooks R, Grulke CM, Ozkaynak H. SHEDS-HT: [An Integrated Probabilistic Exposure Model for Prioritizing Exposures to Chemicals with Near-Field and Dietary Sources](#), Env. Sci. & Tech 2014 48(21):12750-12759 [Exit](#)

Goldsmith MR, Grulke CM, Chang DT, Transue T, Little S, Rabinowitz JR, Tornero-Velez R. [DockScreen: A database of in silico biomolecular interactions to support computational toxicology](#), Dataset Paper in Science 2014 ArticleID:421693 [Exit](#)

View more research publications by [Chris Grulke](#).

**Education:**

- B.S.E., University of Michigan, Ann Arbor, MI; Chemical Engineering, 2003
- Ph.D., University of North Carolina at Chapel Hill; Pharmaceutical Science, Medicinal Chemistry, and Biophysics, 2011

**Professional Experience:**

- EPA Special Accomplishment Award, 2013
- NERL Exposure Science Excellence Award, 2013
- HEASD Paper of the Year Award, 2013