Grace Patlewicz, Ph.D.

SENIOR SCIENCE ADVISOR

CONTACT INFORMATION

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PROFESSIONAL PROFILE

Dr. Grace Patlewicz is a Computational Toxicologist specializing in mammalian toxicity with industrial and regulatory experience in North America and Europe. Dr. Patlewicz has led innovative research programs for developing and applying computational chemistry to identify chemical features associated with specific biological interactions or modes of action, enabling prediction of specific toxicity manifestations of environmental and industrial chemicals. Dr. Patlewicz also leverages computational chemistry principles to develop tools that chemical regulators, researchers, and practitioners can use as adjuncts to modes of action in risk assessment, as well as to weigh the hazard, pharmacokinetic, and exposure-related properties of new and legacy chemicals.

Dr. Patlewicz's research interests have focused on developing and applying (Q)SARs and read-across for regulatory purposes. She has chaired various industry groups and has contributed to technical guidance for (Q)SARs, chemical categories, and Adverse Outcome Pathways (AOPs) under various Organisation for Economic Co-operation and Development (OECD) work programs. Before joining ToxStrategies, Dr. Patlewicz started her toxicology career at Unilever United Kingdom before moving to the European Commission Joint Research Centre in Italy and then to DuPont and the Environmental Protection Agency (EPA) in the United States. She is an Adjunct Professor in the Department of Environmental Sciences and Engineering (ESE) at the University of North Carolina (UNC), Chapel Hill. She has published extensively in the peer-reviewed literature and has presented nationally and internationally at scientific conferences and meetings.

EDUCATION AND DEGREES EARNED

2007	Ph.D. (*cum laude)*, Organic Chemistry, University of Santiago de Compostela, Galicia, Spain
2000	Post-graduate diploma, Management, Henley College, Oxfordshire, UK
1996	M.Sc., Toxicology, University of Surrey, Guildford, UK
1994	B.Sc. (Hons), Chemistry, University of Manchester, Manchester, UK, *first class*

CERTIFICATIONS

2022-Present	Certified Professional Data Scientist, DataCamp, Sept. 2022; renewed Sept. 2024

SOFTWARE AND COMPUTER SKILLS

QSAR/Modelling Software and Tools

OECD QSAR Toolbox
TIMES
Catalogic
VEGA
Toxtree
Toxmatch
Derek & Meteor Nexus
BioTransformer
EPIWIN
ECOSAR
T.E.S.T
Generalized Read-Across (GenRA)

Programming Skills

Python – proficient
R – working knowledge
KNIME
SQL
Mongo
Linux – bash
Docker
Git
Quarto

Technical Proficiencies

Machine learning - Scikit-learn
Deep learning - PyTorch
Web application development - Shiny

PROFESSIONAL ASSOCIATIONS

2016-Present	Society of Toxicology
2015-2024	American Society of Cellular and Computational Toxicology
2015-2020	Society of the Advancement of AOPs (former President)

SELECTED PROFESSIONAL EXPERIENCE

Read-across

- Developed an algorithmic data-driven read-across approach known as Generalized Read-Across (GenRA) to transition from expert driven subjective assessments.
- Established the baseline performance for GenRA for binary read-across predictions of repeated dose toxicity endpoints using a combination of chemical and bioactivity features.
- Actualized GenRA as a public web-based application initially as a module within the EPA CompTox Chemicals Dashboard and subsequently as a standalone tool (https://comptox.epa.gov/genra/) and python package genra-py.

Chemical categories (PFAS)

- Developed an approach for categorizing PFAS as part of the EPA National PFAS Testing Strategy (NTS) first published October 2021 (https://www.epa.gov/assessing-and-managing-chemicals-under-tsca/national-pfas-testing-strategy).
- Refined the approach in light of OSCPP needs and updated it with mechanistic information from NAM assays. Operationalized the categories as a predictive model.
- Developed a prototype python Shiny app to demonstrate how new PFAS could be profiled and assigned into one of the terminal structural categories derived. Prototype is available at patlewig.shinyapps.io/pfas_poc/. The model is also available as an API within the EPA Cheminformatics Modules.

Chemical categories (other)

- Developed a categorization scheme to select ~300 representative substances for testing in NAMs drawn from the TSCA active inventory as part of the EPA OSCPP-ORD New Chemicals Collaborative Research Program (NCCRP).
- Developed a python package to profile substances into one of the New Chemicals Categories (NCC) that is in use by OSCPP New Chemicals. This scheme is available as an API within the EPA Cheminformatics Modules.
- Collaborated with ECHA to publish a machine learning approach to assign chemicals into one of ECHA's Assessment of Regulatory Needs (ARN) groupings. Developed a python package to profile substances into one of the ARN groupings. This scheme is available as an API within the EPA Cheminformatics Modules.

PROFESSIONAL DEVELOPMENT AND SERVICE

2019-Present	Editorial Board Member, *Computational Toxicology*
2019-2022	Editor-in-Chief, *Computational Toxicology* and *Informatics for Frontiers in Toxicology*
2018-Present	Editorial Board Member, *Medicine and Public Health*
2017-Present	Editorial Board Member, *Environmental Health Perspectives*
2014-Present	Editorial Board Member, *ALTEX*
2011-2021	Editorial Board Member, *SAR and QSAR in Environmental Research*
2019-2025	Chair and EPA NCCT (now CCTE) Representative, ICCVAM Acute Toxicity Working Group (ATWG)
2019-2023	Chair and EPA NCCT (now CCTE) Representative, ICCVAM Read-Across Working Group (RAWG)
2020-2022	Member, European Food Standards Agency (EFSA) Read-Across Workgroup
2022-2025	Co-chair and Member, OECD Drafting Grouping Guidance Workgroup
2018-2021	Host and Organizer, 19th International Workshop on QSAR in Environmental Health and Science
2019-2022	EC/ECB Representative, OECD Ad Hoc QSAR Group
2019-2022	EC/ECB Representative, QSAR Working Group (Sub-Group to the TC-NES)
2019-2022	SEAC/Unilever Representative, Business Industry Advisory Committee (BIAC), OECD QSAR Group
2019-2022	SEAC/Unilever Representative, LHASA Deductive Estimation of Risk from Existing Knowledge (DEREK) Collaborative Group
2014-2015	Committee Member, National Academy of Sciences (NAS) Committee on Acute Hazards Associated with Military Exposures
2014	Invited Expert, CMP Committee Meeting for Health and Environmental Canada
2014	DuPont/BIAC Representative, OECD Steering Committee for a Workshop on the Development of IATA
2012-2014	DuPont Representative, CEFIC LRI B14 Skin Sensitization Project: Chemical Applicability Domain of the Local Lymph Node Assay (LLNA)
2013-2014	DuPont Representative, CEFIC LRI AIMT-4 Project: Moving DECO to OECD
2014	DuPont Representative: Advancing AOPS for Integrated Toxicology and Regulatory Applications
2014-2016	DuPont/BIAC / EPA NCCT Representative, OECD Expert Drafting Group for the Development of IATA for Skin Sensitization
2012-2014	Chair, BIAC AOP Workgroup
2008-2014	DuPont/BIAC Representative, OECD Expert Group on Molecular Screening and Toxicogenomics
2012-2014	Chair and DuPont Representative, CEFIC LRI Read-Across Team
2008-2014	Chair, American Chemistry Council (ACC) Computational Profiling Workgroup

2008-2014	DuPont/BIAC Representative, OECD Toolbox Management Group
2007-2014	Moderator of Alttox.org. *Awarded "Moderator of the Quarter, July 2008*
2010-2012	Chair and DuPont Representative, ECETOC Taskforce for Category Approaches, Read-Across, QSAR
2010-2012	Chair and DuPont Representative, CEFIC LRI Organizing Committee for the ECHA/CEFIC LRI Workshop on Read-Across
2008-2011	DuPont Representative, Scientific Advisory Board for the EU OSIRIS Project

SELECTED PUBLICATIONS

Patlewicz G, Judson, Paul Friedman K, Wetmore BA, DeVito MJ, Harrill JA, Carstens KE, Houck KA, et al. 2026. Insights derived from testing a library of per- and polyfluoroalkyl substances (PFAS) in a battery of new approach methods (NAMs). J Toxicol Environ Health B 29(1):1-69; doi: 10.1080/10937404.2025.2521615.

Patlewicz GY, Mihalchik AL. 2026. Revisiting the Threshold of Toxicological Concern: A computational framework for structural classification, cross-scheme comparison and opportunities for refinement. Comput Toxicol 39(Sept):100443; doi: 10.1016/j.comtox.2026.100443.

Patlewicz GY, Mihalchik AL, East A, Borghoff SJ, Thompson CM. 2026. Investigating the feasibility of deriving new environmentally relevant thresholds of Toxicological Concern (TTCs) from estimated chronic human equivalent benchmark dose ($eBMD_{HED}$) values. Comput Toxicol 38(June):100417; doi: 10.1016/j.comtox.2026.100417.

Wambaugh JF, Sipes NS, Padilla Mercado G, Arnot JA, Bertato L, Brown TN, Chirico N,..., **Patlewicz G**, et al. 2026. Collaborative evaluation of in silico predictions for high throughput toxicokinetics. Toxicol In Vitro 110(Jan):106150; doi: 10.1016/j.tiv.2025.106150.

Hagan B, Groff L, **Patlewicz G**, Shah. 2025. Toward metabolic similarity in read-across: A case study using graph convolutional networks to predict genotoxicity outcomes. Chem Res Toxicol 38(6):1122-1133; doi: 10.1021/acs.chemrestox.5c00120.

Hagan B, Shah I, **Patlewicz G**. 2025. Can graph similarity metrics be helpful for analogue identification as part of a read-across approach? Comput Toxicol 34(June):100353; doi: 10.1016/j.comtox.2025.100353.

Hughes MF, DeVito MJ, **Patlewicz G**, Thomas RS, Adams LD, Ambroso JL, Yang X, Upadhyay BG, et al. 2025. Immunotoxicity of four per- and polyfluoroalkyl substances following 28-day oral repeat dosing in rats assessed by the anti-sheep red blood IgM response. Toxics 13(6):490; doi: 10.3390/toxics13060490.

Karamertzanis PG, Rasenberg M, Shah I, **Patlewicz G**. 2025. Modelling in vitro mutagenicity using multi-task deep learning and REACH data. Chem Res Toxicol 38(8):1382-1407; doi: 19.1021/acs.chemrestox.5c00152.

Kenyon EM, DeVito MJ, **Patlewicz G**, Adams LD, Thomas RS, Ambroso JL, Yang X, Blake JC, et al. 2025. Subchronic toxicity of four per- and polyfluoroalkyl substances by oral exposure in Sprague Dawley rats. Toxics 13(7):524; doi: 10.3390/toxics13070524.

Leary A, Shah I, **Patlewicz G**. 2025. An exploration of the use of hybrid fingerprints in Generalized Read-Across and their impact on predictive performance for selected *in vivo* toxicity outcomes. Comput Toxicol 34(June):100349; doi: 10.1016/j.comtox.2025.100349.

Nyffeler J, Harris FR, Willis C, Byrd G, Blackwell B, Escher BI, Kasparek A, Nichols J,..., **Patlewicz G**, et al. 2025. A combination of high-throughput in vitro and in silico new approach methods (NAMs) for ecotoxicology hazard assessment for fish. Environ Toxicol Chem 44(9):2599-2621; doi: 10.1093/etojnl/vgae083.

Patlewicz G, Charest N, Ross A, Bledsoe HC, Vidal J, Faramarzi S, Hagan B, Shah I. 2025. Building a compendium of expert driven read-across cases to facilitate an analysis of the contribution that different similarity contexts play in read-across performance. Comput Toxicol 35(Sept):100366; doi: 10.1016/j.comtox.2025.100366.

Patlewicz G, Williams AJ, Adams M, Shah I, Paul-Friedman K. 2025. A cheminformatics workflow to select representative TSCA chemicals for New Approach Methodology (NAM) screening. Chem Res Toxicol 38(1):129-144; doi: 10.1021/acs.chemrestox.4c00367.

Payton A, Hickman, Chappel J, Roell KR, Koval LA, Eaves LA, Chou CK,..., **Patlewicz G**, et al. 2025. TAME 2.0: Expanding and improving online data science training for environmental health research. Front Toxicol 7(Feb 12):1535098; doi: 10.3389/ftox.2025.1535098.

Banerjee A, Kar S, Roy K, **Patlewicz G**, Charest N, Benfenati E, Cronin MTD. 2024. Molecular similarity in chemical informatics and predictive toxicity modeling: From quantitative read-across (q-RA) to quantitative read-across structure-activity relationship (q-RASAR) with the application of machine learning. Crit Rev Toxicol 54(9):659-684; doi: 10.1080/10408444.2024.2386260.

Firman JW, Boobis A, Hollnagel HM, Kaiser S, Lovell DP, Moretto A, Muller S,..., **Patlewicz G**. 2024. Evaluating the consistency of judgements derived through both *in silico* and expert application of the Cramer classification scheme. Food Chem Toxicol 194(Dec):115070; doi: 10.1016/j.fct.2024.115070.

Groff L, Williams A, Shah I, **Patlewicz G**. 2024. MetSim: Integrated programmatic access and pathway management for xenobiotic metabolism simulators. Chem Res Toxicol 37(5):685-697; doi: 10.1021/acs.chemrestox.3c00398.

Judson RS, Smith D, DeVito M, Wambaugh JF, Wetmore BA, Paul Friedman K, **Patlewicz G**, Thomas RS, et al. 2024. A comparison of in vitro points of departure with human blood levels for per- and polyfluoroalkyl substances (PFAS). Toxics 12(4):271; doi: 10.3390/toxics12040271.

Karamertzanis P, **Patlewicz G**, Sannicola M, Paul-Friedman K, Shah I. 2024. Systematic approaches for the encoding of chemical groups: A case study. Chem Res Toxicol 37(4):600-619; doi: 10.1021/acs.chemrestox.3c00411.

Patlewicz G, Judson RS, Williams AJ, Butler T, Barone Jr. S, Carstens K, Cowden J, Dawson JD, et al. 2024. Development of chemical categories for per- and polyfluoroalkyl substances (PFAS) and the proof-of-concept approach to the identification of potential candidates for tiered toxicological testing and human health assessment. Comput Toxicol 131(Sep 1):100327; doi: 10.1016/j.comtox.2024.100327.

Patlewicz G, Karamertzanis P, Paul-Friedman K, Sannicola M, Shah I. 2024. A systematic analysis of read-across within REACH registration dossiers. Comput Toxicol 30(June):100304; doi: 10.1016/j.comtox.2024.100304.

Shirke AV, Radke EG, Lin C, Blain R, Vetter N, Lemeris C, Hartman P,.., **Patlewicz G**, et al. 2024. Expanded systematic evidence map for hundreds of per- and polyfluoroalkyl substances (PFAS) and comprehensive PFAS human health dashboard. Environ Health Perspect 132(2):026001; doi: 10.1289/EHP134.

Tate T, **Patlewicz G**, Shah I. 2024. A comparison of machine learning approaches for predicting hepatotoxicity potential using chemical structure and targeted transcriptomic data. Comput Toxicol 29(March):100301; doi: 10.1016/j.comtox.2024.100301.

Adams M, Hilde H, Chang D, Richard A, Williams AJ, Shah I, **Patlewicz G**. 2023. Development of a CSRML version of the Analog Identification Methodology (AIM) fragments and their evaluation within the Generalized Read-Across (GenRA) approach. Comput Toxicol 25(Feb):100256; doi: 10.1016/j.comtox.2022.100256.

Bowden A, Escher S, Rose J, Sadekar N, **Patlewicz G**, O'Keeffe L, Bury D, Hewitt NJ, et al. 2023. Workshop report: Challenges faced in developing inhalation thresholds of Toxicological Concern (TTC) – State of the science and next steps. Regul Toxicol Pharmacol 142(Aug):105434; doi: 10.1016/j.yrtph.2023.105434.

Boyce M, Favela KA, Bonzo JA, Chao A, Lizarraga L, Moody LR, Owens EO, **Patlewicz G**, et al. 2023. Identifying xenobiotic metabolites with in silico prediction tools and LCMS suspect screening analysis. Front Toxicol 5(Jan 18):1051483; doi: 10.3389/ftox.2023.1051483.

Carstens KE, Freudenrich T, Wallace K, Choo S, Carpenter A, Smeltz M, Clifton MS,..., **Patlewicz G**, et al. 2023. Evaluation of per- and polyfluoroalkyl substances (PFAS) in vitro toxicity testing for developmental neurotoxicity. Chem Res Toxicol 36(3):402–419; doi: 10.1021/acs.chemrestox.2c00344.

Houck K, Paul Friedman K, Feshuk M, **Patlewicz G**, Smeltz M, Clifton S, Wetmore BA, Velichko S, et al. 2023. Evaluation of 147 perfluoroalkyl substances for immunotoxic and other (patho)physiological activities through phenotypic screening of human primary cells. ALTEX 40(2):248–270; doi: 10.14573/altex.2203041.

Lizarraga L, Suter GW, Lambert JC, **Patlewicz G**, Zhao JQ, Dean JL, Kaiser P. 2023. Advancing the science of a read-across framework for evaluation of data poor chemicals incorporating systematic and new approach methods. Regul Toxicol Pharm 137(Jan):105293; doi: 10.1016/j.yrtph.2022.105293.

Maloney EM, Villeneuve DL, Jensen KM, Blackwell BR, Kahl MD, Poole ST, Vitense K, Feifarek, DJ, **Patlewicz G**, et al. 2023. Evaluation of complex mixture toxicity: An experimental and database-driven analysis in the Milwaukee estuary (WI, USA) using whole-mixture and component-based evaluation methods. Environ Toxicol Chem 42(6):1229-1256; doi: 10.1002/etc.5571.

Nyffeler J, Willis C, Harris FR, Foster MJ, Chambers B, Culbreth M, Brockway RE,..., **Patlewicz G**, et al. 2023. Application of cell painting for chemical hazard evaluation in support of screening-level chemical assessments. Toxicol Appl Pharmacol 468(June 1):116513; doi: 10.1016/j.taap.2023.116513.

Patlewicz G, Paul Friedman K, Houck K, Zhang L, Huang R, Xia M, Brown J, Simmons SO. 2023. Evaluating the utility of a high throughput thiol-containing fluorescent probe to screen for reactivity: A case study with the Tox21 library. Comput Toxicol 26(May):100271; doi: 10.1016/j.comtox.2023.100271.

Patlewicz G, Shah I. 2023. Towards systematic read-across using Generalized Read-Across (GenRA). Comput Toxicol 25(Feb):100258; doi: 10.1016/j.comtox.2022.100258.

Richard AM, Lougee R, Adams M, Hidle H, Yang C, Rathman J, Magdziarz T, Bienfait B, Williams AJ, **Patlewicz G**. 2023. A new CSRML structure-based fingerprint method for profiling and categorizing per- and polyfluoroalkyl substances (PFAS). Chem Res Toxicol 36(3):508–534; doi: 10.1021/acs.chemrestox.2c00403.

Beal MA, Gagne M, Kulkarni SA, **Patlewicz G**, Thomas RS, Barton-Maclaren TS. 2022. Implementing in vitro bioactivity to modernize priority setting of chemical inventories. ALTEX 39(1):123-139; doi: 10.14573/altex.2106171.

Boyce M, Meyer B, Grulke C, Lizarraga L, **Patlewicz G**. 2022. Comparing the performance and coverage of selected in silico (liver) metabolism tools related to reported studies in the literature to inform analogue selection in read-across: A case study. Comput Toxicol 21(Feb):100208; doi: 10.1016/j.comtox.2021.100208.

Carlson LM, Angrish M, Shirke AV, Radke EG, Schulz B, Kraft A, Judson RS, **Patlewicz G**, et al. 2022. Systematic evidence map for over one hundred and fifty per- and polyfluoroalkyl substances (PFAS). Environ Health Perspect 130(5):56001; doi: 10.1289/EHP10343.

Cronin MTD, Bauer FJ, Bonnell M, Campos B, Ebbrell DJ, Firman JW, Gutsell S, Hodges G, **Patlewicz G**, et al. 2022. A scheme to evaluate structural alerts to predict toxicity–Assessing confidence by characterizing uncertainties. Regul Toxicol Pharmacol 135(Nov):105249; doi: 10.1016/j.yrtph.2022.105249.

Foster MJ, **Patlewicz G**, Shah I, Haggard DE, Judson RS, Paul Friedman K. 2022. Evaluating structure-based activity in a high throughput assay for steroid biosynthesis. Comput Toxicol 24(Nov):100245; doi: 10.1016/j.comtox.2022.100245.

Karmaus A, Mansouri K, To K, Blake B, Fitzpatrick J, Strickland J, **Patlewicz G**, Allen D, et al. 2022. Evaluation of variability across rat acute oral systemic toxicity studies. Toxicol Sci 188(1):34-47; doi: 10.1093/toxsci/kfac042.

Nicolas CI, Linakis MW, Minto MS, Mansouri K, Clewell RA, Yoon M, Wambaugh JF, **Patlewicz G**, et al. 2022. Estimating provisional margins of exposure for data poor chemicals using high throughput computational methods. Front Pharmacol 13(Oct 7):980747; doi: 10.3389/fphar.2022.980747.

Patlewicz G. 2022. Editorial: Reflections of the QSAR2021 meeting. Comput Toxicol 22(May):100221; doi: 10.1016/j.comtox.2022.100221.

Patlewicz G, Nelms MN, Rua D. 2022. Evaluating the utility of the Threshold of Toxicological Concern (TTC) and its exclusions in the biocompatibility assessment of extractable chemical substances from medical devices. Comput Toxicol 24(Nov):100246; doi: 10.1016/j.comtox.2022.100246.

Patlewicz G, Richard AM, Williams AJ, Judson RS, Thomas RS. 2022. Towards reproducible structure-based chemical categories for PFAS to inform and evaluate toxicity and toxicokinetic testing. Comput Toxicol 24(Nov):100250; doi: 10.1016/j.comtox.2022.100250.

Patlewicz G, Worth AP, Yang C, Zhu T. 2022. Editorial: Advances and refinements in the development and application of threshold of toxicological concern. Front Toxicol 4(Apr 28):882321; doi: 10.3389/ftox.2022.882321.

Ponder J, Rajagopal R, Singal M, Baker N, **Patlewicz G**, Roggen E, Cochrane S, Sullivan K. 2022. “In Litero” screening. Retrospective evaluation of clinical evidence to establish a reference list of human chemical respiratory sensitizers. Front Toxicol 4(Jul 15):916370; doi: 10.3389/ftox.2022.916370.

Richard AM, Hidle H, **Patlewicz G**, Williams AJ. 2022. Identification of branched and linear forms of PFOA and potential precursors: a user-friendly SMILES structure-based approach. Front Environ Sci 10(Mar 24):865488; doi: 10.3389/fenvs.2022.865488.

Roell K, Koval LE, Boyles R, **Patlewicz G**, Ring C, Rider CV, Ward-Caviness C, Reif D, et al. 2022. Development of the intelligence and machine learning toolkit (TAME) for introductory data science, chemical-biological analyses, predictive modelling, and database mining for environmental health research. Front Toxicol 4(Jun 22):893924; doi: 10.3389/ftox.2022.893924.

Shah I, Bundy J, Chambers B, Everett L, Haggard D, Harrill J, Judson R, Nyffeler J, **Patlewicz G**. 2022. Navigating transcriptomic connectivity mapping workflows to link chemicals with bioactivities. Chem Res Toxicol 35(11):1929-1949; doi: 10.1021/acs.chemrestox.2c00245.

Williams AJ, Gaines LG, Grulke CM, Lowe CN, Sinclair G, Samano V, Thillainadarajah I, Meyer B, **Patlewicz G**, Richard AM. 2022. Assembly and curation of list of per- and polyfluoroalkyl substances (PFAS) to support environmental science research. Front Environ Sci 10(Apr 5):1-13; doi: 10.3389/fenvs.2022.850019.

Zwickl CM, Graham JC, Holly RA, Bassan A, Ahlberg E, Amberg A, Anger LT,.., **Patlewicz G**, et al. 2022. Principles and procedures for assessment of acute toxicity incorporating in silico methods. Comput Toxicol 24(Nov):100237; doi: 10.1016/j.comtox.2022.100237.

Brozek JL, Canelo-Aybar C, Akl EA, Bowen JM, Bucher J, Chiu WA, Cronin M, Djulbegovic B,..., **Patlewicz G**, et al. 2021. GRADE Guidelines 30: The GRADE approach to assessing the certainty of modeled evidence—An overview in the context of health decision-making. J Clin Epidemiol 129(Jan):138-150; doi: 101016/j.jclinepi.2020.09.018.

Houck KA, **Patlewicz G**, Richard A, Williams AJ, Smeltz M, Clifton, MS, Wetmore B, Medvedev A, Makarov SS. 2021. Bioactivity profiling of per- and polyfluoroalkyl substances identifies potential toxicity pathways related to molecular structure. Toxicology 457(June 15):152789; doi: 10.1016/j.tox.2021.152789.

Mansouri K, Karmaus A, Fitzpatrick J, **Patlewicz G**, Pradeep P, Alberga D et al. 2021. CATMoS: Collaborative acute toxicity modeling suite. Environ Health Perspect 129(4):47013; doi: 10.1289/EHP8495.

Patlewicz G, Dean J, Gibbons C, Judson R, Keshava N, Vegosen L, Martin T, Pradeep P, et al. 2021. Integrating publicly available information to screen potential candidates for chemical prioritization under the Toxic Substances

Control Act: A proof of concept case study using genotoxicity and carcinogenicity. Comput Toxicol 20(Nov):100185; doi: 10.1016/j.comtox.2021.100185.

Pradeep P, Judson RS, DeMarini DM, Keshava N, Martin TM, Dean J, Gibbons CF,..., **Patlewicz G**. 2021. An evaluation of existing QSAR models and structural alerts and development of new ensemble models for genotoxicity using a newly compiled experimental dataset. Comput Toxicol 18(May):100167; doi.org/10.1016/j.comtox.2021.100167.

Rovida C, Escher SE, Herzler M, Bennekou SH, Kamp H, Kroese DE, Maslankiewicz L, Moné MJ, **Patlewicz G**, et al. 2021. NAM-supported read-across: From case studies to regulatory guidance in safety assessment. ALTEX 38(1):140-150; doi: 10.14573/altex.2010062.

Shah I, Tate T, **Patlewicz G**. 2021. Generalized Read-Across prediction using genra-py. Bioinformatics 37(19):3380-3381; doi: 10.1093/bioinformatics/btab210.

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Nelms MD, Karmaus AL, **Patlewicz G**. 2020. An evaluation of the performance of selected (Q)SARs/expert systems for predicting acute oral toxicity. Comput Toxicol 16(Nov):100135; doi: 10.1016/j.comtox.2020.100135.

Nelms MD, **Patlewicz G**. 2020. Derivation of new threshold of toxicological concern values for exposure via inhalation for environmentally-relevant chemicals. Front Toxicol 2:580347; doi: 10.3389/ftox.2020.580347.

Patlewicz G. 2020. Navigating the minefield of computational toxicology and informatics: Looking back and charting a new horizon. Front Toxicol 2:2; doi: 10.3389/ftox.2020.00002.

Pradeep P, **Patlewicz G**, Pearce R, Wambaugh J, Wetmore B, Judson R. 2020. Using chemical structure information to develop predictive models for in vitro toxicokinetic parameters to inform high-throughput risk-assessment. Comput Toxicol 16(Nov):100136; doi: 10.1016/j.comtox.2020.100136.

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Helman G, **Patlewicz G**, Shah I. 2019. Quantitative prediction of repeat dose toxicity values using GenRA. Regul Toxicol Pharmacol 109(Dec):104480; doi: 10.1016/j.yrtph.2019.104480.

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Becker RA, Paul KB, Simon TW, Marty S, **Patlewicz G**, Rowland JC. 2015. An exposure:activity profiling method for interpreting high-throughput screening data for estrogenic activity—Proof of concept. Regul Toxicol Pharmacol 71(3):398-408; doi: 10.1016/j.yrtph.2015.01.008.

Patlewicz G, Ball N, Boogaard P, Becker RA, Hubesch B. 2015. Building scientific confidence in the development and evaluation of read-across. Regul Toxicol Pharmacol 72(1):117-133; 10.1016/j.yrtph.2015.03.015.

Patlewicz G, Simon T, Rowlands JC, Budinsky R, Becker RA. 2015. Proposing a scientific confidence framework to help support the application of adverse outcome pathways for regulatory purposes. Regul Toxicol Pharmacol 71(3):463-477; doi: 10.1016/j.yrtph.2015.02.011. (*Top 10 Paper for RASS Award at SOT 2016*)

Petkov P, **Patlewicz G**, Schultz TW, Honma M, Todorov M, Kotov S, Dimitrov SD, Donner EM, Mekenyan OM. 2015. A feasibility study: Can information collected to classify for mutagenicity be informative in predicting carcinogenicity? Regul Toxicol Pharmacol 72(1):17-25; doi: 10.1016/j.yrtph.2015.03.003.

BOOK CHAPTERS, REPORTS, AND OTHER DOCUMENTS

Brennan A, Chang D, Cowden J, Davidson-Fritz S, Dean J, Devito M, Ford J,..., **Patlewicz G**, et al. 2024. EPA Transcriptomic Assessment Product (ETAP) for Perfluoro-3-Methoxypropanoic Acid. EPA/600/X-24/066. U.S. Environmental Protection Agency: Washington, DC; doi: 10.23645/epacomptox.25352962.

Chang D , Cowden J, Davidson-Fritz S, Dean J, Devito M, Everett L, Harrill A,.., **Patlewicz G**, et al. 2024. Scientific Studies Supporting Development of Transcriptomic Points of Departure for EPA Transcriptomic Assessment Products (ETAPs). EPA/600/X-23/084. U.S. Environmental Protection Agency: Washington, DC; doi: 10.23645/epacomptox.25365550.

Lizarraga LE, **Patlewicz G**, Dean JL II, Zhao QJ, Kaiser JP. 2022. Provisional Peer-Reviewed Toxicity Values for 2,3-Toluenediamine (CASRN 2687-25-4).

Lizarraga LE, **Patlewicz G**, Dean JL II, Zhao QJ, Kaiser JP. 2022. Provisional Peer-Reviewed Toxicity Values for 3,4-Toluenediamine (CASRN 496-72-0).

Contributor. 2021. Work contribution to the A Proof-of-Concept Case Study Integrating Publicly Available Information to Screen Candidates for Chemical Prioritization under the Toxic Substances Control Act (TSCA. October.

Contributor. 2021. Work contribution to the OECD/UNEP Global PFCs Group - PFAS terminology project. Reconciling Terminology of the Universe of Per- and Polyfluoroalkyl Substances: Recommendations and Practical Guidance. Series on Risk Management No. 61. August.

Fourches D, Williams AJ, **Patlewicz G**, Shah I, Grulke C, Wambaugh J, Richard A, Tropsha A. 2018. Computational tools for ADMET profiling. Chapter 8 in: *Computational Toxicology: Risk Assessment for Chemicals*, Ed Ekins, ed. Wiley. pp. 211-244; doi: 10.1002/9781119282594.ch8.

Contributor. 2016. Work contribution to the OECD Series on Testing and Assessment: Guidance Document on the Reporting of Defined Approaches to be used within Integrated Approaches to Testing and Assessment for Skin Sensitization, Number 256. October.

Contributor. 2016. Work contribution to the OECD Series on Testing and Assessment: Guidance Document on the Reporting of Defined Approaches to be used within Integrated Approaches to Testing and Assessment, Number 255. October.

Contributor. 2015. Work contribution as Committee member to the National Academies of Sciences (NAS) report entitled "Application of Modern Toxicology Approaches for Predicting Acute Toxicity for Chemical Defense." July.

Contributor. 2014. Work contribution as drafting group member to the OECD Series on Testing and Assessment: Guidance Document for Describing Non-Guideline *in vitro* Test Methods, Number 211. December.

Contributor. 2014. Work contribution as drafting group member to the OECD Series on Testing and Assessment: Guidance on Grouping of Chemicals. April.

Contributor. 2007. Work contribution as drafting group member to ECHA Guidance on Information Requirements and Chemical Safety Assessment Endpoint specific guidance (Chapter R.7a) – Skin and Respiratory Sensitization.

Contributor. 2007. Work contribution as drafting group member and co-chair to ECHA Guidance on Information Requirements and Chemical Safety Assessment (Q)SARs and grouping of chemicals (Chapter R.6).

Patlewicz G, Worth A. 2008. Review of Data Sources, QSARs and Integrated Testing Strategies for Skin Sensitization. EUR 23225 EN.

Contributor. 2004. Work contribution as drafting group member to the OECD Series on Testing and Assessment Number 49: The Report from The Expert Group On (Quantitative) Structure-Activity Relationships [(Q)SARs] on the Principles for the Validation of (Q)SARs.

Contributor. 2007. Work contribution to the OECD Series on Testing and Assessment Number 80: Guidance on Grouping of Chemicals. Paris: OECD.

Patlewicz G, Gallegos Saliner A, Pavan M, Worth A, Benigni R, Aptula A, Bassan A, Bossa C, et al. 2007. Chemical Similarity and Threshold of Toxicological Concern (TTC) Approaches. Report of an ECB Workshop held in Ispra, November 2005. EUR 22657 EN.

Worth A, Bassan A, Fabjan E, Gallegos Saliner A, Netzeva T, Patlewicz G, Pavan M, Tsakovska I. 2007. The Use of Computational Methods in the Grouping and Assessment of Chemicals - Preliminary Investigations. EUR 22941 EN.

Worth AP, Patlewicz G, Eds. 2007. A Compendium of Case Studies that helped to shape the REACH Guidance on Chemical Categories and Read Across. EUR 22481 EN.

Gallegos Saliner A, Patlewicz G, Worth AP. 2006. Review of Literature-Based Models for Skin and Eye Irritation and Corrosion. EUR 22320 EN.

Gallegos A, Patlewicz G, Worth AP. 2005. A Similarity Based Approach for Chemical Category Classification. EUR 21867 EN.

Worth AP, Bassan A, Gallegos A, Netzeva TI, Patlewicz G, Pavan M, Tsakovska I, Vracko M. 2005. The Characterization of (Quantitative) Structure-Activity Relationships: Preliminary Guidance. EUR 21866 EN*.

**This ECB report was written to provide preliminary guidance on how to characterize (Q)SARs according to the OECD validation principles. The report was developed further by the OECD QSAR Group and, following adoption by the OECD Member Countries and the Commission, was published as an OECD Guidance Document (February 2007) see: https://one.oecd.org/document/env/jm/mono(2007)2/en/pdf*

SELECTED PRESENTATIONS AND POSTERS

Nagyal M, Kopanska K, Rovida C, Antignac E, Barton-Maclaren T, Congreave I, Escher SE,..., **Patlewicz G**, et al. From thresholds to odds: AI-enhanced applications of the threshold of toxicological concern (TTC) in modern risk assessment. Oral Session 3, Poster OR-12, American Society for Cellular and Computational Toxicology (ASCCT) 15th Annual Meeting, Durham, NC, October 28, 2026.

Patlewicz G, Mihalchik AL. Refinement of the threshold of toxicological concern (TTC): A computational framework for cross-scheme comparison of TTC values. Poster Session I, Poster 24, American Society for Cellular and Computational Toxicology (ASCCT) 15th Annual Meeting, Durham, NC, October 27, 2026.

East A, Klaren W, Wikoff D, **Patlewicz G**. Identifying potential co-exposures with food additives using data mining and machine learning approaches across EPA's Consumer Product Database (CPDat). Abstract M-36, Poster Session, International Society of Exposure Science (ISES) 2026 Annual Meeting, Vancouver, BC, Canada, October 5, 2026.

Fitch S, Lozy F, Mitchell C, **Patlewicz G**, Wood A. Use of new approach methodologies in the safety assessment of dietary supplements—Parts one and two. Webinar series, Council for Responsible Nutrition (CRN), Washington, DC, May 2026.

Patlewicz G, Mihalchik A, Thompson CM, East A, Borghoff S. Investigating the feasibility of deriving a new environmentally relevant Thresholds of Toxicological Concern (TTCs) from estimated human equivalent benchmark dose ($eBMD_{HED}$) values. Abstract 4013, Society of Toxicology 65th Annual Meeting, San Diego, CA, March 2026.

ASCCT Meeting. Three poster presentations, Research Triangle Park, NC, September 2024.

EPA NAM Tools Training event. Facilitator for GenRA session, Research Triangle Park, NC, May 24-25, 2024.

Society of Toxicology 63rd Annual Meeting. Session chair and presenter / two poster presentations / booth demonstrator for GenRA, March 10-14, 2024.

OSCPP PFAS Stakeholder Workshop. Invited presentation, February 13-15, 2024.

OSCPP Fragrance Stakeholder Meeting. Invited participant, February 30, 2024.

CalEPA. Invited presenter on read-across approaches, January 11, 2024.

OECD Working Meeting for the Drafting of Grouping Guidance, Co-chair, November 12-14, 2023.

Lecture on QSARs/Read-across, UNC Chapel Hill, NC, October 2023.

SciPy Annual Meeting, Austin, TX, July 10-26, 2023.

QSAR 2023. Keynote speaker / two presentations / three posters / panelist, Copenhagen, Denmark, June 4-9, 2023.

ASCCT. Three poster presentations, Chapel Hill, NC, October 2022.

GenRA Webinar NAMs Training. Primary trainer and presenter of GenRA, May 2022.

Korea SOT Meeting. Invited speaker, May 12, 2021.

QSAR and Read-across in Toxicological Assessments. Invited speaker, April 28, 2021 *(highest rated of all speakers presenting in the event based on attendees).*

Cefic-LRI / ILSI Europe Digital Workshop on "Carcinogen Dose-Response Database for Threshold of Toxicological Concern (TTC)". Moderator, April 19-21, 2021.

Society of Toxicology 60th Annual Meeting. Session chair, Virtual, March 12-26, 2021.

Cosmetics Europe Inhalation TTC Workshop. Invited presenter, November 3-4, 2020.

NAS Workshop on Federal Government Human Health PFAS Research. Respondent, October 26-27, 2020.

ASCCT. Organiser and presenter for the EPA CompTox Chemicals Dashboard training, Virtual, October 23, 2020.

ASCCT. Poster presenter, Virtual, Oct 21-22, 2020.

AWMA: The Science of PFAS: Chemistry, Health, and Multimedia Measurements. Invited speaker, September 15, 2020.

Society of Toxicology 59th Annual Meeting. Platform speaker, Virtual, March 15-19, 2020.

Personal Care Council. Invited keynote speaker, Philadelphia, PA, October 30, 2019.

PANWAT Regional Chapter Meeting. Invited keynote speaker, Boise, ID, October 6-7, 2019.

IUTOX 15th International Congress of Toxicology. CE presenter and platform presenter, Honolulu, HI, July 15-18, 2019.

Toxforum Annual Meeting. Invited speaker, Alexandria, VA, July 10, 2019.

ICCA LRI Workshop. Invited Speaker, Stresa, Italy, June 18-20, 2019.

EU ToxRisk Workshop on Read-across. Invited presenter / rapporteur / organizing committee member, Helsinki, Finland, May 21-23, 2019.

Cal EPA PFAS Workshop. Invited speaker, Oakland, CA, May 1-3, 2019.

APRCA—Accelerating the Pace of Risk Assessment. Platform presenter, Ottawa, ON, October 10-11, 2018.

Texas A&M. Invited lecturer, College Station, TX, April 30, 2018.

ICCVAM Workshop: Predictive Models for Acute Oral Systemic Toxicity. Member of organizing committee / presenter / facilitator/rapporteur of breakout session, National Institutes of Health, Bethesda, MD, April 11-12, 2018.

North Carolina State University. Invited speaker, April 4, 2018.

ACS National Meeting. Chair of session / two platform presentations / co-author on one other platform presentation, New Orleans, LA, March 18-22, 2018.

Society of Toxicology 57th Annual Meeting. Co-author on five poster presentations / platform presenter, San Antonio, TX, March 11-15, 2018.

48th Annual Meeting for EMGS. Invited speaker, Raleigh, NC, September 9-13, 2017.

10th World Congress for Animal and Alternatives in Life Sciences (WC10). Invited speaker and chair / two platform presentations / co-author on one other platform presentation / three poster presentations, Seattle, WA, August 20-24, 2017.

OpenTox ISA. Invited speaker, Duke University, Durham, NC, July 12-13, 2017.

ACS Spring Meeting. Co-author on one platform / one poster presentation, San Francisco, CA, April 2-6, 2017.

Society of Toxicology 56th Annual Meeting. Session chair / co-author on three poster presentations / CE presenter. Baltimore, MD, March 12-16, 2017.

Workshop: State of the Science on Alternatives to Animal Testing and Integration of Testing Strategies for Food Safety Assessment: Co-hosted by US FDA, CFSAN and ILSI NA Technical Committee on Food and Chemical Safety. Invited speaker, College Park, MD, February 28, 2017.

2017 GlobalChem Meeting, Invited speaker, Washington DC, February 22-24, 2017.

41st Winter Meeting of the Toxicology Forum. Invited speaker, Washington DC, February 6-8, 2017.

5th Annual Meeting of the ASCCT. Session chair / co-author on four posters, Research Triangle Park, NC, September 29-30, 2016.

Alternative Approaches for Acute Inhalation Toxicity Testing to Address Global Regulatory and Non-regulatory Data Requirements. Moderator, Bethesda, MD, September 22-23, 2016.

EU ToxRisk/Tox21 Workshop. Invited participant, Mainz, Germany, September 12-14, 2016.

SOT FDA Colloquia on the State of the Art in the Cramer Classification Scheme and Threshold of Toxicological Concern. Invited speaker, College Park, MD, March 29, 2016.

Globalchem 2016. Invited speaker, Washington DC, March 22-24, 2016.

Society of Toxicology 55th Annual Meeting. Session co-chair / platform presenter / co-author on three poster presentations, New Orleans, LA, March 13-17, 2016.

CAAT Good Read-across Practice (GRAP) Guidance Workshop. Invited speaker, College Park, MD, March 1, 2016.

JRC Expert Meeting on Pre- and Pro-haptens. Invited speaker, Ispra, Italy, November 10-11, 2015.

Cosmetic Europe Workshop on Informing and Supporting Mechanisms for Cosmetic Chemical Space – Driving Clarity on Needs for New Approaches to Safety Assessment. Invited speaker, Brussels, June 2-3, 2015.

Society of Toxicology 54th Annual Meeting. Co-author on two poster presentations, San Diego, March 22-26, 2015.

OpenTox 2015. Session chair, Baltimore, MD, February 10-12, 2015.