

Curriculum Vitae - Trevor N. Brown, Ph.D.

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<https://tnbrowncontam.github.io/>

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EDUCATION

Ph.D. - University of Toronto - Toronto ON, Canada - 2006-2011

Department of Chemistry, Environmental Chemistry

Supervisor: Frank Wania

Thesis Title: Automated Methods in Chemical Risk Assessment

B.Sc. - Thompson Rivers University - Kamloops BC, Canada - 2001-2006

Major in Environmental Chemistry, Co-operative Education Endorsement

Student research supervisor: Nelaine Mora-Diez

PROFESSIONAL EXPERIENCE

Contract Researcher - Halifax NS, Canada - 2019-present

Subcontractor and collaborator with ARC Arnot Research and Consulting

Physical Scientist - Fisheries and Oceans Canada - Halifax NS, Canada - 2016-2019

Centre for Offshore Oil, Gas and Energy Research, Supervisor: Thomas King

Created prediction methods for the chemical properties of oil components

Provided scientific advice and assistance to projects undertaken by the group

Assisted with the writing of scientific reports

Assisted with administrative tasks

Contract Researcher - Halifax NS, Canada - 2012-2016

Subcontractor and collaborator with ARC Arnot Research and Consulting

Co-applicant or project team member on several funded grant applications

Main role was creating prediction methods for chemical properties (QSARs)

Advised and assisted with dataset selection and quality control

Undertook other scientific activities such as manuscript writing

Postdoc - Dalhousie University - Halifax NS, Canada - 2014-2015

Department of Chemistry, Supervisor: Russell Boyd

Manuscript writing

Postdoc - Helmholtz Centre for Environmental Research (UFZ) - Leipzig, Germany - 2011-2014

Department of Analytical Environmental Chemistry, Supervisor: Kai-Uwe Goss
Created prediction methods for chemical properties (QSARs)
Modelling and prediction of chemical distribution and clearance processes in humans
Advising and collaborating on various internal UFZ research projects
Co-supervising a Ph.D. student modelling fish embryo chemical exposure

Graduate Student Researcher - University of Toronto - Toronto ON, Canada - 2006-2011
Department of Chemistry, Environmental Chemistry, Supervisor: Frank Wania
Designed, created and modified mass balance chemical environmental fate models
Screened datasets for chemical hazard by applying modelling and chemoinformatics tools
Developed a method for creating predictive models of chemical properties (QSARs)
Assisted other students with lab work, field work and chemical fate modelling

Teaching Assistant - University of Toronto Scarborough - Toronto ON, Canada - 2007-2010
Assisted with graduate level class on chemical fate modelling, graded assignments and exams
Demonstrated first year chemistry laboratories and graded lab reports

Student Researcher - Thompson Rivers University - Kamloops BC, Canada - 2005-2006
Performed quantum chemistry calculations with commercial software
Undertook other research related tasks such as coding and writing manuscripts

Analytical Chemist - ALS Environmental - Vancouver BC, Canada - 2004
Performed sample extraction and clean-up of air, water and soil samples
Analyzed samples for total petroleum hydrocarbons using GC-FID

AWARDS AND SCHOLARSHIPS

Humboldt Research Fellowship for Postdoctoral Researchers, Germany - 2012-2013
Ontario Graduate Student Award (OGS) - 2010-2011
Teaching Reduction Award, University of Toronto, Department of Chemistry - 2008, 2009
Thompson Rivers University, Student Travel Award - 2005, 2006
NSERC Undergraduate Student Research Award - 2004

PEER REVIEWED PUBLICATIONS

Brown T.N., Armitage J.M., Sangion A., Arnot J.A.; Improved prediction of PFAS partitioning with PPLFERS and QSPRs. Environ. Sci.: Process. Impacts, 2024, In Press.

Brown T.N., Sangion A., Arnot J.A.; Identifying uncertainty in physical–chemical property estimation with IFSQSAR. J. Cheminform., 2024, 16, 65.

Zhang Z., Sangion A., Wang S., Gouin T., **Brown T.N.**, Arnot J.A., Li L.; Chemical Space Covered by Applicability Domains of Quantitative Structure–Property Relationships and Semiempirical Relationships in Chemical Assessments. *Environmental Science & Technology*, 2024, 58 (7), 3386-3398.

Zhang Z., Wang S., **Brown T.N.**, Sangion A., Arnot J.A., Li L.; Modeling sorption of environmental organic chemicals from water to soils. *Water Research X*, 2024, 22, 100219.

Celsie A.K.D., Parnis J.M., **Brown T.N.**; Metrics for estimating vapour pressure deviation from ideality in binary mixtures. *SAR and QSAR in Environmental Research*, 2023, 34 (11), 943-961.

Zhang Z., Sangion A., S Wang, Gouin T., **Brown T.N.**, Arnot J.A., Li L.; Hazard vs. exposure: Does it make a difference in identifying chemicals with persistence and mobility concerns? *Water Research*, 2023, 245, 120610.

Ding Y., Hayward S.J., Westgate J.N., **Brown T.N.**, Lei Y.D., Wania F.; Legacy and current-use pesticides in Western Canadian mountain air: Influence of pesticide sales, source proximity, and altitude. *Atmospheric Environment*, 2023, 308, 119882.

Arnot J.A., Toose L., Armitage J.M., Sangion A., Looky A., **Brown T.N.**, Li L., Becker R.A.; Developing an internal threshold of toxicological concern (iTTC). *Journal of Exposure Science & Environmental Epidemiology*, 2022, 32 (6), 877-884.

Brown T.N.; QSPRs for predicting equilibrium partitioning in solvent–air systems from the chemical structures of solutes and solvents. *Journal of Solution Chemistry*, 2022, 51 (9), 1101-1132

Brown T.N.; Empirical regressions between system parameters and solute descriptors of polyparameter linear free energy relationships (PPLFERs) for predicting solvent-air partitioning. *Fluid Phase Equilibria*, 2021, 540, 113035.

Brown T.N., Armitage J.M., Arnot J.A.; Application of an iterative fragment selection (IFS) method to estimate entropies of fusion and melting points of organic chemicals. *Mol. Inform.*, 2019, 38, 1800160.

Hussain B.A., Westgate J.N., Hayward S.J., Shunthirasingham C., **Brown T.N.**, Hung H., Lei Y.D., Wania F.; Polycyclic aromatic hydrocarbons and polychlorinated biphenyls in soils and atmosphere of Western Canadian mountains: The role of source proximity, precipitation, forest cover and mountain cold-trapping. *Atmosph. Environ. X*, 2018, 1, 100004.

Undeman E., Brown T.N., McLachlan M.S., Wania F.; Who in the world is most exposed to polychlorinated biphenyls? Using models to identify highly exposed populations. *Environ. Res. Lett.*, 2018, 13, 064036.

Larisch W., **Brown T.N.**, Goss K.U.; A toxicokinetic model for fish including multiphase sorption features. *Environ. Toxicol. Chem.*, 2017, 36, 1538-1546.

Arp H.P.H., **Brown T.N.**, Berger U., Hale S.E.; Ranking REACH registered neutral, ionizable and ionic organic chemicals based on their aquatic persistency and mobility. *Environ. Sci. Proc. Imp.*, 2017, 19, 939-955.

Chen Y., Hermens J.L.M., Jonker M.T.O., Arnot J.A., Armitage J.M., **Brown T.N.**, Nichols J.W., Fay K.A., Droge S.T.J.; Which molecular features affect the intrinsic hepatic clearance rate of ionizable organic chemicals in fish? *Environ. Sci. Technol.*, 2016, 50, 12722-12731.

Brown T.N., Armitage J.M., Egeghy P., Kircanski I., Arnot J.A.; Dermal permeation data and models for the prioritization and screening-level exposure assessment of organic chemicals. *Environ. Int.*, 2016, 94, 424-435.

McLachlan M.S., Kierkegaard A., Radke M., Sobek A., Malmvärn A., Alsberg T., Arnot J.A., **Brown T.N.**, Wania F., Breivik K., Xu S.; Using model-based screening to help discover known environmental contaminants. *Environ. Sci. Technol.*, 2014, 48, 7264-7271.

Arnot J.A., **Brown T.N.**, Wania F.; Estimating screening-level organic chemical half-lives in humans. *Environ. Sci. Technol.*, 2014, 48, 723-730.

Brown T.N.; Predicting hexadecane-air equilibrium partition coefficients (L) with a group contribution approach constructed from high-quality data. *SAR QSAR Environ. Res.*, 2014, 25, 51-71.

Zhang X., **Brown T.N.**, Ansari A., Yeun B., Kitaoka K., Kondo A., Lei Y.D., Wania F.; Effect of wind on the chemical uptake kinetics of a passive air sampler. *Environ. Sci. Technol.*, 2013, 47, 7868-7875.

Endo S., **Brown T.N.**, Goss K.-U.; General model for estimating partition coefficients to organisms and their tissues using the biological compositions and polyparameter linear free energy relationships. *Environ. Sci. Technol.*, 2013, 47, 6630-6639.

Goss K.-U., **Brown T.N.**, and Endo S.; Elimination half-life as a metric for the bioaccumulation potential of chemicals in aquatic and terrestrial food chains. *Environ. Toxicol. Chem.* 2013, 32, 1663-1671.

Armitage J.M., Choi S.-D., Meyer T., **Brown T.N.**, Wania F.; Exploring the role of shelf sediments in the Arctic Ocean in determining the Arctic contamination potential of neutral organic contaminants. *Environ. Sci. Technol.* 2013, 47, 923-931.

Arnot J.A., **Brown T.N.**, Wania F., Breivik K., McLachlan M.S.; Prioritizing Chemicals and Data Requirements for Screening-Level Exposure and Risk Assessment. *Environ. Health Perspect.* 2012, 120, 1565-1570.

Brown T.N., Arnot J.A., and Wania F.; Iterative Fragment Selection: A Group Contribution Approach to Predicting Fish Biotransformation Half-Lives. *Environ. Sci. Technol.* 2012, 46, 8253-8260.

Breivik K., Arnot J.A., **Brown T.N.**, McLachlan M.S., Wania F.; Screening organic chemicals in commerce for emissions in the context of environmental and human exposure. *J. Environ. Monit.*, 2012, 14, 2028-2037.

Undeman E., **Brown T.N.**, Wania F., McLachlan M.S.; The Susceptibility of Human Populations to Environmental Exposure to Organic Contaminants. *Environ. Sci. Technol.* 2010, 44, 6249-6255.

Zhang X., **Brown T.N.**, Wania F., Heimstad E.S., Goss K.-U.; Assessment of Chemical Screening Outcomes Based on Different Partitioning Property Estimation Methods. *Environ. Int.* 2010, 36, 514-520.

Brown T.N. and Wania F.; Development and Exploration of an Organic Contaminant Fate Model Using Poly-Parameter Linear Free Energy Relationships. *Environ. Sci. Technol.* 2009, 43, 6676-6683.

Brown T.N. and Wania F.; Screening Chemicals for the Potential to be Persistent Organic Pollutants: A Case Study of Arctic Contaminants. *Environ. Sci. Technol.* 2008, 42, 5202-5209.

Brown T.N. and Mora-Diez N.; Computational determination of aqueous pK_a values of protonated benzimidazoles (part 1). *J. Phys. Chem. B* 2006, 110, 9270-9279.

Brown T.N. and Mora-Diez N.; Computational determination of aqueous pK_a values of protonated benzimidazoles (part 2). *J. Phys. Chem. B* 2006, 110, 20546-20554.

REPORTS AND OTHER WORK

Brown T.N., IFSQSAR python package, <https://github.com/tnbrowncontam/ifsqsar>.

Armitage J.M., Arnot J.A., **Brown T.N.**, Sangion A., Toose L.; Identification of Surrogates for Estimating the Biopartitioning of Organic Chemicals. Prepared for U.K. Environment Agency, 2024.

Brown T.N., Li L., Zhang X., Sangion A., Toose L., Wania F., Arnot J.A.; Developing guidance and recommendations for using overall fate and monitoring data in a weight-of-evidence for assessing petroleum hydrocarbon persistence under REACH. Prepared for Concawe Task Force(s) Biological Effects Measures (STF-32), Ecology Group (EG), 2021.

Arnot J.A., **Brown T.N.**, Toose L., Sangion A., Armitage J.M.; Modernize Health Canada's Consumer and Industrial/Aquaculture Release Models and Incorporate them into the EAS-E Suite Platform. Prepared for New Substances Assessment and Control Bureau, Healthy Environments and Consumer Safety Branch, Health Canada, 2021.

Ryan A.S., Wohlgeschaffen G., Jahan N., Niu H., Ortmann A.C., **Brown T.N.**, King T.L., Clyburne J.; State of Knowledge on Fate and Behaviour of Ship-Source Petroleum Product Spills: Volumes 1-5, Halifax Canada, Fisheries and Oceans Canada, Canadian Manuscript Report of Fisheries and Aquatic Sciences 3176, 2019.

Ulrich N., Endo S., **Brown T.N.**, Watanabe N., Bronner G., Abraham M.H., Goss K.-U.; UFZ-LSER database v 3.2.1 [Internet], Leipzig, Germany, Helmholtz Centre for Environmental Research-UFZ, 2017, Available from <http://www.ufz.de/lserd>.

SELECTED CONFERENCE PRESENTATIONS

Brown T.N., Sangion A., Arnot J.A. (2019) A new database and preliminary QSARs for environmentally relevant biodegradation half-lives. Society of Environmental Toxicology and Chemistry (SETAC) North America, Toronto, Canada. Poster presentation.

Brown T.N. (2019) Modelling the SARA Fractionation of Oil Components. 102nd Canadian Chemistry Conference and Exhibition, Quebec City, Canada. Oral presentation.

Brown T.N. (2018) Predicting dilbit weathering with a simulated molecular composition. AMOP Technical Seminar on Environmental Contamination and Response, Victoria, Canada. Poster presentation.

Brown T.N., Armitage J.M., Arnot J.A. (2015) Addressing uncertainty in sub-cooled liquid property estimation: Applications for chemical activity calculations. Society of Environmental Toxicology and Chemistry (SETAC) North America, Salt Lake City, U.S.A. Poster presentation.

Brown T.N. (2015) Unifying data from chemistry, biology, and human health fields of science within a single framework to improve PBTK modelling. Society of Environmental Toxicology and Chemistry (SETAC) Europe, Barcelona, Spain. Poster presentation.

Brown T.N., Armitage J.M., Arnot J.A. (2014) Exploring fragment-based QSARs to predict the equilibrium partitioning of ionogenic organic chemicals to biologically relevant media. Society of Environmental Toxicology and Chemistry (SETAC) North America, Vancouver, Canada. Oral presentation.

Brown T.N., Stenzel A., Goss. K-U (2013) Assessing the reliability of QSAR predictions for structurally complex chemicals. American Chemical Society (ACS) National Meeting & Exposition, Indianapolis, U.S.A. Oral presentation.

Brown T.N., Goss K.-U. (2012) New physiology-based pharmacokinetic model for predicting mammalian tissue distribution of pesticides. Society of Environmental Toxicology and Chemistry (SETAC) World, Berlin, Germany. Oral presentation.

Brown T.N., Arnot J.A. (2012) Prediction of environmental and biological degradation half-lives with quantitative structure activity relationships. Society of Environmental Toxicology and Chemistry (SETAC) World, Berlin, Germany. Poster presentation.

Brown T.N., Arnot J.A., Wania F. (2011) Generation of 2D QSARs for Properties Relevant to Chemical Prioritization. Society of Environmental Toxicology and Chemistry (SETAC) North America, Boston, U.S.A. Oral presentation.

Brown T.N., Arnot J.A. Wania F. (2011) Evaluating Overall Degradability of Chemicals with QSARs, Society of Environmental Toxicology and Chemistry (SETAC) North America, Boston, U.S.A. Oral presentation.

Brown T.N., Kumarappah A., Wania F. (2011) Long range transport versus source region exposure potential: effect of dynamic climactic scenarios. Society of Environmental Toxicology and Chemistry (SETAC) Europe, Milan, Italy. Poster presentation.

Brown T.N., Undeman E., Hong A., Mclachlan M.S., Wania F. (2011) Simulated trophic magnification factors: sensitivity analysis and comparison to human exposure modelling. Society of Environmental Toxicology and Chemistry (SETAC) Europe, Milan, Italy. Poster presentation.

Brown T.N., Arnot J. and Wania F. (2010) Prediction of metabolic biotransformation half-lives using iterative fragment selection (IFS). Environmental Transformation of Organic Compounds (TransCon2010), Monte Verità, Switzerland. Oral presentation.

Brown T.N., Arnot J. and Wania F. (2010) Prediction of metabolic biotransformation half-lives using iterative fragment selection (IFS). Society of Environmental Toxicology and Chemistry (SETAC) Europe, Seville, Spain. Poster presentation.

Brown T.N. and Wania F. (2010) Investigating the time resolution of variable environmental forcing parameters and their effect on chemical fate modelling. Society of Environmental Toxicology and Chemistry (SETAC) Europe, Seville, Spain. Poster presentation.

Brown T.N. and Wania F. (2009) Implementation of poly-parameter linear free energy relationships in a multimedia fate model. 12th European Association for Chemical and Molecular Sciences (EuCheMS) International Conference on Chemistry and the Environment (ICCE), Stockholm, Sweden. Oral presentation.

Brown T.N. and Wania F. (2009) Screening chemicals for the potential to be POPs, 12th European Association for Chemical and Molecular Sciences (EuCheMS) International Conference on Chemistry and the Environment (ICCE), Stockholm, Sweden. Poster Presentation.

Brown T.N. and Wania F. (2009) Controlled indoor experiments on the wind speed dependence of contaminant uptake in XAD-based passive air samplers. 12th European Association for Chemical and Molecular Sciences (EuCheMS) International Conference on Chemistry and the Environment (ICCE), Stockholm, Sweden. Poster Presentation.

Brown T.N. and Wania F. (2008) Screening chemicals for the potential to be persistent organic pollutants: a case study of Arctic contaminants. Society of Environmental Toxicology and Chemistry (SETAC) Europe, Warsaw, Poland. Oral presentation.

Brown T.N., Wania F, Breivik K., and Goss K.-U. (2008) Testing a dynamic multi-media model describing environmental phase partitioning with poly-parameter linear free energy relationships. Society of Environmental Toxicology and Chemistry (SETAC) Europe, Warsaw, Poland. Poster presentation.

FUNDED GRANT APPLICATIONS

Co-applicant: European Chemical Industry Council Long-Range Research Initiative (CEFIC-LRI): ECO54: Developing a tiered modeling framework in support of risk assessment of chemical substances associated with mobility concerns, 2020 - 2024.

Co-applicant: European Chemical Industry Council Long-Range Research Initiative (CEFIC-LRI): B22: Tiered Methods for Quantifying Exposure to Complex Substances (TMEx-Complex), 2020 - 2022.

Co-applicant: Concawe Task Force Biological Effects Measures (STF-32), Ecology Group (EG): Developing guidance and recommendations for using overall fate and monitoring data in a weight-of-evidence for assessing petroleum hydrocarbon persistence under REACH, 2020 – 2021.

Co-applicant: European Chemical Industry Council Long-Range Research Initiative (CEFIC-LRI): ECO30: Expanding the applicability domain of the chemical activity approach for hazard and risk assessment, 2015 - 2017.

Co-applicant: American Chemistry Council Long-Range Research Initiative (ACC-LRI): Improving exposure models and integrating exposure and risk information for high-throughput chemical screening (prioritization) and higher tiered assessments, 2015 - 2017.

Co-applicant: European Chemical Industry Council Long-Range Research Initiative (CEFIC-LRI): ECO21: Improving the performance and expanding the applicability of a mechanistic bioconcentration model for ionogenic organic compounds (IOCs) in fish, 2013 - 2015.

Project team member: American Chemistry Council Long-Range Research Initiative (ACC-LRI): Developing, applying and evaluating models for screening level chemical exposure and risk assessment, 2012 - 2014.

Project team member: Environment Canada: Developing databases and models for mammalian biotransformation rate and dietary assimilation efficiency for improved bioaccumulation assessment, 2012 - 2013.

Project team member: Unilever: Expanding the evaluation of the chemical activity hypothesis for toxicity and risk assessment, 2012 - 2014.