Nigel Greene, Ph.D.

SENIOR CONSULTANT

CONTACT INFORMATION

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PROFESSIONAL PROFILE

Dr. Nigel Greene is a computational and drug discovery toxicologist in ToxStrategies' Pharmaceuticals practice. With over thirty years of experience working in computational ADME and toxicology, secondary pharmacology, cheminformatics, medicinal chemistry, new approach methodologies (NAMs), and drug discovery, Dr. Greene is a recognized international expert in his field. His specialties include machine learning (ML) and artificial intelligence (AI), protein modeling, and protein-ligand docking and their applications.

Dr. Greene is a demonstrated leader whose skill with cross-functional team collaboration and working with diverse groups within matrixed management systems has guided pharmaceutical organizations to success. Prior to joining ToxStrategies, Dr. Greene served in senior leadership positions in several large pharmaceutical firms, where he managed ML and AI teams including bioinformatics, drug discovery and preclinical safety teams, providing strategy for early discovery safety testing and other global research and development programs.

EDUCATION AND DEGREES EARNED

Ph.D., Organometallic Chemistry, University of Leeds, Leeds, West Yorkshire, England

B.S., Chemistry and Computational Science, University of Leeds, Leeds, West Yorkshire, England (subsidiary subjects in Mathematics and Management Studies)

Bachelor of Dental Surgery (BChD), University of Leeds, Leeds, West Yorkshire, England (incomplete)

PROFESSIONAL ASSOCIATIONS

2025–Present American College of Toxicology

2003–Present Society of Toxicology

PROFESSIONAL SERVICE/ACTIVITIES

- Associate Editor, *Toxicological Sciences* journal, 2023-present.
- Elected to the Board of Trustees of Lhasa Ltd. in 2002. Elected Deputy Chair of the Board of Trustees in June 2011 and took over as Chair of the Board in June 2013 until June 2015. Responsible for the governance and oversight for a $10M turnover charitable organization that employs more than 80 staff.
- Member, Lhasa Ltd. Scientific Advisory Board, 2005-2015.
- President, Computational Toxicology Specialty Section of the Society of Toxicology, 2022-2023.
- Served on the National Academy of Science committees sponsored by the United States Environmental Protection Agency (EPA), Food and Drug Administration (FDA), and National Institutes of Health (NIH) for:
  - A Framework to Guide the Selection of Chemical Alternatives, 2013-2014.
  - Using 21st Century Science to Improve Risk-Related Evaluations, 2015-2017.

SELECTED MANUSCRIPTS

Hanser T, Ahlberg E, Amberg A, Anger LT, Barber C, Brennan RJ, Brigo A,..., **Greene N**, et al. 2025. Data-driven federated learning in drug discovery with knowledge distillation. Nat Mach Intell 7(Mar):423–436.

Seal S, Trapotsi MA, Spjuth O, Singh S, Carreras-Puigvert J, **Greene N**, Bender A, Carpenter AE. 2025. Cell painting: A decade of discovery and innovation in cellular imaging. Nat Meth 22(2):254-268.

Seal S, Trapotsi M, Subramanian V, Spjuth O, **Greene N**, Bender A. 2025. PKSmart: An open-source computational model to predict in vivo pharmacokinetics of small molecules. J Cheminform 17(1):147.

Bak A, Burlage R, **Greene N**, Nambiar P, Lu X, Templeton A. 2024. Accelerating drug product development and approval: Early development and evaluation. Pharm Res 41(1):1-6.

Gawehn E, **Greene N**, Miljković F, Obrezanova O, Subramanian V, Trapotsi M, Winiwarter S. 2024. Perspectives on the use of machine learning for ADME prediction at AstraZeneca. Xenobiotica 54(7):368-378.

Kenyon MO, Martin M, Martin EA, Brandstetter S, Wegesser T, **Greene N**, Harvey J. 2024. Deriving acceptable limits for non-mutagenic impurities in medicinal products–Durational adjustments. Regul Toxicol Pharmacol 150(June):105644.

Snodin DJ, Trejo-Martin A, Ponting DJ, Smith GF, Czich A, Cross K, Custer L,... **Greene N**, et al. 2024. Mechanisms of nitrosamine mutagenicity and their relationship to rodent carcinogenic potency. Chem Res Toxicol 37(2):181-198.

Wright PSR, Briggs KA, Thomas R, Smith GF, Maglennon G, Mikulskis P, Chapman M, **Greene N**, et al. 2023. Statistical analysis of preclinical interspecies concordance of histopathological findings in the eTOX database. Regul Toxicol Pharmacol 138(Feb):105308.

Wright PSR, Smith GF, Briggs KA, Thomas R, Maglennon G, Mikulskis P, Chapman M, **Greene N**, et al. 2023. Retrospective analysis of the potential use of virtual control groups in preclinical toxicity assessment using the eTOX database. Regul Toxicol Pharmacol 138(Feb):105309.

Obrezanova O, Martinsson A, Whitehead T, Mahmoud S, Bender A, Miljković F, Grabowski P,..., **Greene N**. 2022. Prediction of in vivo pharmacokinetic parameters and time–exposure curves in rats using machine learning from the chemical structure. Molec Pharm 19(5):1488-1504.

Bassan A, Alves VM, Amberg A, Anger LT, Auerbach S, Beilke L, Bender A..., **Greene N**, et al. 2021. *In silico* approaches in organ toxicity hazard assessment: Current status and future needs in predicting liver toxicity. Computation Toxicol 20(Nov):100187.

Giblin KA, Basili D, Afzal AM, Rosenbrier-Ribeiro L, **Greene N**, Barrett I, Hughes SJ, Bender A. 2021. New associations between drug-induced adverse events in animal models and humans reveal novel candidate safety targets. Chem Res Toxicol 34(2):438-451.

Miljković F, Martinsson A, Obrezanova O, Williamson B, Johnson M, Sykes A, Bender A, **Greene N**. 2021. Machine learning models for human in vivo pharmacokinetic parameters with in-house validation. Molec Pharm 18(12):4520-4530.

Sturm N, Mayr A, Le Van T, Chupakhin V, Ceulemans H, Wegner J, Golib-Dzib J-F,..., **Greene N**, et al. 2020. Industry-scale application and evaluation of deep learning for drug target prediction. J Cheminform 12(1):26.

DeGeorge J, Robertson S, Butler L, Derzi M, Stoch SA, Diaz D, Hartke J,..., **Greene N**. 2018. An industry perspective on the 2017 EMA guideline on first-in-human and early clinical trials. Clin Pharm Ther 103(4):566-569.

Rusyn I, **Greene N**. 2018. The impact of novel assessment methodologies in toxicology on green chemistry and chemical alternatives. Toxicol Sci 161(2):276-284.

Svensson F, Zoufir A, Mahmoud S, Afzal AM, Snit S, Giblin KA, Clements PJ,..., **Greene N**, et al. 2018. Information-derived mechanistic hypotheses for structural cardiotoxicity. Chem Res Toxicol 31(11):1119-1127.

Winiwarter S, Ahlberg E, Watson E, Oprisiu I, Mogemark M, Noeske T, **Greene N**. 2018. In silico ADME in drug design–Enhancing the impact. ADMET DMPK 6(1):15-33.

Butler LD, Guzzie-Peck P, Hartke J, Bogdanffy MS, Will Y, Diaz D, Mortimer-Cassen E,..., **Greene N**, et al. 2017. Current nonclinical testing paradigms in support of safe clinical trials: An IQ Consortium DruSafe perspective. Regul Toxicol Pharmacol 87(Sup 3):S1-S15.

Sanz F, Pognan F, Steger-Hartmann T, Díaz C, Cases M, Pastor M, Marc P,..., **Greene N**, et al. 2017. Legacy data sharing to improve drug safety assessment: the eTOX project. Nat Rev Drug Discov 6(12):811-812.

Barber C, Cayley A, Hanser T, Harding A, Heghes C, Vessey JD, Werner S,..., **Greene N**. 2016. Evaluation of a statistics-based Ames mutagenicity QSAR model and interpretation of the results obtained. Regul Toxicol Pharmacol 76(Apr):7-20.

Williams RV, Amberg A, Brigo A, Coquin L, Giddings A, Glowienke S, **Greene N**, et al. 2016. It's difficult, but important, to make negative predictions. Regul Toxicol Pharmacol 76(Apr):79-86.

Greene N, Dobo KL, Kenyon MO, Cheung J, Munzner J, Sobol Z, Sluggett G, Zelesky T, et al. 2015. A practical application of two in silico systems for identification of potentially mutagenic impurities. Regul Toxicol Pharmacol 72(2):335-49.

Greene N, Pennie W. 2015. Computational toxicology: Friend or foe? Toxicol Res 4(5):1159-1172.

Shah F, Leung L, Barton HA, Will Y, Rodrigues AD, **Greene N**, Aleo MD. 2015. Setting clinical exposure levels of concern for drug-induced liver injury (DILI) using mechanistic in vitro assays. Toxicol Sci 147(2):500-14.

Steinbach T, Gad-McDonald S, Kruhlak N, Powley M, **Greene N**. 2015. (Q)SAR: A tool for the toxicologist. Int J Toxicol 34(4):352-4.

Shah F, Hashimoto T, Segall MD, **Greene N**. 2014. Finding the rules for successful drug optimization. Drug Discov Today 18(13-14):659-666.

Shah F, Louise-May S, **Greene N**. 2014. Chemotypes sensitivity and predictivity of in vivo outcomes for cytotoxic assays in THLE and HepG2 cell lines. Bioorg Med Chem Lett 24(12):2753-2757.

Zhang L, McHale CM, **Greene N**, Snyder R, Rich IN, Aardema MJ, Roy S, Pfuhler S, et al. 2014. Emerging approaches in predictive toxicology. Environ Mol Mutagen 55(9):679-88.

Davis PA, Wiegers TC, Roberts PM, King BL, Lay JM, Lennon-Hopkins K, Sciaky D,..., **Greene N**, et al. 2013. A CTD–Pfizer collaboration: Manual curation of 88 000 scientific articles text mined for drug–disease and drug–phenotype interactions. Database 2013(Nov 28):bat080.

Naven RT, Swiss R, Klug-McLeod J, Will Y, **Greene N**. 2013. The development of structure-activity relationships for mitochondrial dysfunction: Uncoupling of oxidative phosphorylation. Toxicol Sci 131(1):271-278.

Shah F, **Greene N**. 2013. Analysis of Pfizer compounds in EPA's ToxCast chemicals-assay space. Chem Res Toxicol 27(1):86-98.

Sutter A, Amberg A, Boyer S, Brigo A, Contrera JF, Custer LL, Dobo KL,..., **Greene N**, et al. 2013. Use of in silico systems and expert knowledge for structure-based assessment of potentially mutagenic impurities. Regul Toxicol Pharmacol 67(1):39-52.

Dobo KL, **Greene N**, Fred C, Glowienke S, Harvey JS, Hasselgren C, Jolly R, Kenyon MO, et al. 2012. In silico methods combined with expert knowledge rule out mutagenic potential of pharmaceutical impurities: An industry survey. Regul Toxicol Pharmacol 62(3):449-455.

Naven RT, **Greene N**, Williams RV. 2012. Latest advances in computational genotoxicity prediction. Exp Opin Drug Metabol 8(12):1579-87.

Wang X, **Greene N**. 2012. Comparing measures of promiscuity and exploring their relationship to toxicity. Molec Inform 3(2):145-159. *Awarded Best Paper of 2012 by the editors of Molecular Informatics*.

Enayetallah AE, Ziemek D, Leininger MT, Randhawa R, Yang J, Manion TB, Mather DE,..., **Greene N**, et al. 2011. Modeling the mechanism of action of a DGAT1 inhibitor using a causal reasoning platform. PLoS One 6(11):e27009.

Greene N, Song M. 2011. Predicting in vivo safety characteristics using physicochemical properties and in vitro assays. Fut Med Chem 3(12):1503-1511.

Greene N, Aleo MD, Louise-May S, Price DA, Will Y. 2010. Using an in vitro cytotoxicity assay to aid in compound selection for in vivo safety studies. Bioorg Med Chem Lett 20(17):5308-5312.

Greene N, Fisk L, Naven RT, Note RR, Patel ML, Pelletier DJ. 2010. Developing structure-activity relationships for the prediction of hepatotoxicity. Chem Res Toxicol 23(7):1215-1222.

Naven RT, Louise-May S, **Greene N**. 2010. The computational prediction of genotoxicity. Exp Opin Drug Metabol Toxicol 6(7):1-11.

BOOK CHAPTERS

Fisk L, **Greene N**, Naven R. 2018. Physicochemical properties and structural alerts. In: Chen M, Will Y (eds), Drug-Induced Liver Toxicity, Humana: New York, pp. 61-76.

Greene N, Gosink M. 2013. Computational toxicology experience and applications for risk assessment in the pharmaceutical industry. Chapter 10 in: Fowler BA (ed), Computational Toxicology: Methods and Applications. Elsevier-Academic Press, pp. 171-193.

Boyer S, Muthas D, **Greene N**. 2011. Information, informatics and modeling in predictive toxicology. Chapter 5 in: Wilson AG, Rotella D, (eds), New Horizons in Predictive Toxicology: Current Status and Application. RSC Drug Discovery Series, Vol. 12. Royal Society of Chemistry Publishing, pp. 70-100.

ABSTRACTS AND PRESENTATIONS

Greene N. The role of AI in advancing drug discovery. Abstract 1055, Society of Toxicology 65th Annual Meeting, San Diego, CA, March 2026.

Snyder K, **Greene N**, De Nieu M, Anger L, Shah F. Developing predictive models to facilitate interpretation of toxicology study results. Symposium co-chair, Symposium S04, American College of Toxicology (ACT) 46th Annual Meeting, Phoenix, AZ, November 2025.

Bai P, Miljković F, Ge Y, **Greene N**, John B, Lu H. Hierarchical clustering split for low-bias evaluation of drug-target interaction prediction. IEEE International Conference on Bioinformatics and Biomedicine (BIBM); doi: 10.1109/BIBM52615.2021.966915. Houston, TX, December 2021.

Wright PSR, Briggs KA, Thomas R, Smith GF, Maglennon G, Mikulskis P, Chapman M, **Greene N**, Bender A. The impact of pooling animal histopathology control data on the statistical detection of treatment-related findings. Abstract SOC02-05, 56th Congress of the European Societies of Toxicology (EUROTOX 2021). Toxicol Lett 350(Sup):S63, 2021.

Butler L, Guzzie-Peck P, Hartke J, Bogdanffy M, Will Y, Diaz D, Mortimer-Cassen E,.., **Greene N**, et al. Revised draft EMA guidance on early clinical trials: Potential impacts and industry response. Abstract P204, American College of Toxicology 2017 Annual Meeting, Palm Springs, CA, 2017. Int J Toxicol 37(1):75-76, 2018.