

## Antony Williams, Chemist, in EPA's National Center for Computational Toxicology

### [Mailing Address](#)

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**Area of Expertise:** Dr. Williams' present focus at NCCT is as part of the Chemical Safety for Sustainability (CSS) Research Program to develop a cheminformatics architecture for the center. This work has already produced the publicly accessible website, the iCSS Chemistry Dashboard, providing access to chemistry related data for over 700,000 chemicals (<https://comptox.epa.gov/dashboard>).

### Select Publications:

[The development of models to predict melting and pyrolysis point data associated with several hundred thousand compounds mined from PATENTS](#), I.V. Tetko, D.M. Lowe and A.J. Williams, Journal of Cheminformatics 2016, 8:2 doi:10.1186/s13321-016-0113-y [Exit](#)

[Linking High Resolution Mass Spectrometry Data with Exposure and Toxicity Forecasts to Advance High-Throughput Environmental Monitoring](#), J. Sobus, J.E Rager, M.J Strynar, S. Liang; R.L McMahan; A.M Richard, C.M Grulke, J.F Wambaugh, K.K Isaacs, R.J. Judson and A.J Williams, Environmental International, Volume 88, 2016, 269–280, doi: 10.1016/j.envint.2015.12.008 [Exit](#)

[Ambiguity of non-systematic chemical identifiers within and between small-molecule databases](#), S. A. Akhondi, S. Muresan, A.J. Williams, J.A. Kors, Journal of Cheminformatics, 2015, 7:54 doi:10.1186/s13321-015-0102-6 [Exit](#)

[The parallel worlds of open, public and commercial bioactive chemistry data](#), C. Lipinski, N. Litterman, C. Southan, A.J. Williams, A. Clark and S. Ekins, Journal of Medicinal Chemistry, 58 (5), pp 2068–2076, 2015 [Exit](#)

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### Education:

- B.S., Liverpool University, Liverpool, UK; Chemistry, 1985
- Ph.D., University of London, London, UK; Chemistry, 1988

### Professional Experience:

- North Carolina ACS Distinguished Lecturer, 2016
- Microsoft eScience Jim Gray Award, 2012
- Fellow of the Royal Society of Chemistry, 2009
- University of London Bourne Medal for best Chemistry Thesis, 1988
- Morris Ranger Undergraduate scholarship, 1983

### Additional Publications:

[National Center for Biotechnology Information](#) [Exit](#)