

Tox21 Data Challenge 2014

About the Data



([data.jsp](#))

NCATS will provide assay activity data and chemical structures on the Tox21 collection of ~10,000 compounds (Tox21 10K). A collection of compounds independent of the Tox21 10K collection will be used as the test set.

[Get the Data » \(data.jsp\)](#)

The Challenge

The 2014 Tox21 (<http://www.ncats.nih.gov/research/reengineering/tox21/tox21.html>) data challenge is designed to help scientists understand the potential of the chemicals and compounds being tested through the Toxicology in the 21st Century (<http://www.ncats.nih.gov/research/reengineering/tox21/tox21.html>) initiative to disrupt biological pathways in ways that may result in toxic effects.

The goal of the challenge is to "crowdsource" data analysis by independent researchers to reveal how well they can predict compounds' interference in biochemical pathways using only chemical structure data. The computational models produced from the Challenge could become decision-making tools for government agencies in determining which environmental chemicals and drugs are of the greatest potential concern to human health.

[Learn More » \(about.jsp\)](#)

All challenge winners

will receive the opportunity to submit a paper for publication in a special thematic issue of *Frontiers in Environmental Science* (<http://journal.frontiersin.org/researchtopic/2954/tox21-challenge-to-build-predictive-models-of-nuclear-receptor-and-stress-response-pathways-as-media#articles>) and recognition on the NCATS website and via social media.

Key Dates

August 18, 2014

NCATS begins accepting submissions

November 14, 2014

Registration and submission deadline

January 12, 2015

Winners announced

[Register Now » \(registration.jsp\)](#)

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