1.	Record Nr.	UNINA9910227348503321
	Autore	Menghang Xia
	Titolo	Tox21 Challenge to Build Predictive Models of Nuclear Receptor and Stress Response Pathways as Mediated by Exposure to Environmental Toxicants and Drugs
	Pubbl/distr/stampa	Frontiers Media SA, 2017
	Descrizione fisica	1 electronic resource (102 p.)
	Collana	Frontiers Research Topics

Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Sommario/riassunto	Tens of thousands of chemicals are released into the environment every day. High-throughput screening (HTS) has offered a more efficient and cost-effective alternative to traditional toxicity tests that can profile these chemicals for potential adverse effects with the aim to prioritize a manageable number for more in depth testing and to provide clues to mechanism of toxicity. The Tox21 program, a collaboration between the National Institute of Environmental Health Sciences (NIEHS)/National Toxicology Program (NTP), the U.S. Environmental Protection Agency's (EPA) National Center for Computational Toxicology (NCCT), the National Institutes of Health (NIH) National Center for Advancing Translational Sciences (NCATS), and the U.S. Food and Drug Administration (FDA), has generated quantitative high-throughput screening (qHTS) data on a library of 10K compounds, including environmental chemicals and drugs, against a panel of nuclear receptor and stress response pathway assays during its production phase (phase II). The Tox21 Challenge, a worldwide modeling competition, was launched that asks a "crowd" of researchers to use these data to elucidate the extent to which the interference of biochemical and cellular pathways by compounds can be inferred from chemical structure data. In the Challenge participants were asked to model twelve assays related to nuclear receptor and stress response pathways using the data generated against the Tox21 10K compound library as

the training set. The computational models built within this Challenge are expected to improve the community's ability to prioritize novel chemicals with respect to potential concern to human health. This research topic presents the resulting computational models with good predictive performance from this Challenge.