

3 - Predictive Models Used In This Challenge

Guide to Submissions to the NIEHS-NCATS-UNC DREAM Toxicogenetics Challenge

Participants in the [NIEHS-NCATS-UNC DREAM Toxicogenetics Challenge](#) were provided with training data giving a measure of cytotoxicity (EC10) for each of 487 cell lines derived from the [1000 Genomes Project](#).

There were 2 parts to the challenge with separate winners in each category. In [Subchallenge 1](#), the task was to predict toxicity for previously seen compounds in new cell lines, while [Subchallenge 2](#) asked participants to estimate the distribution of toxicity of new compounds across cell lines.

Winning Submissions

Subchallenge 1

The [winning entry for subchallenge 1](#) came from [Tao Wang](#) of the [Yang](#) lab at the [Quantitative Biomedical Research Center](#) at UTSW. [R source code](#) available.

Runners up, [Team CASSIS](#), submitted an entry titled, [Kernel Bilinear Regression for toxicogenetics](#) along with [source code in R](#).

Subchallenge 2

The [winning entry for subchallenge 2](#) also came from [QBRC](#), this time from a team led by [Hao Tang](#). The approach was to cluster compounds then predict based on similarity of new compounds to the clusters. [R source code](#) available.

Participating Teams

Subchallenge 1

Team	Project	Team Members	Organization(s)	Location(s)
amss2012	syn376020	Junfei Zhao, Shihua Zhang	National Center for Mathematics and Interdisciplinary Sciences, Academy of Mathematics and Systems Science, Chinese	Beijing, China

Team	Project	Team Members	Organization(s)	Location(s)
			Academy of Sciences	
bioinfoCIPF	syn2225007	Alicia Amadoz, Patricia Sebastian-Leon, Rosa D. Hernansaiz and Joaquin Dopazo	Computational Genomics Department, Centro de Investigacion Principe Felipe (CIPF)	Valencia, Spain
BorRfLm	syn2223113	Zofia Wiśniewska, Miron Bartosz Kursa	Interdisciplinary Centre for Mathematical and Computational Modelling, University of Warsaw	Warsaw, Poland
CASSIS	syn2224192	Elsa Bernard ^{1,2,3} , Erwan Scornet ^{1,2,3,4} , Yunlong Jiao ^{1,2,3} , Veronique Stoven ^{1,2,3} , Thomas Walter ^{1,2,3} , Jean-Philippe Vert ^{1,2,3}	1 Mines ParisTech, Centre for Computational Biology; 2 Institut Curie; 3 INSERM U900; 4 University Pierre et Marie Curie	Fontainebleau; Paris, France
Charlie's Minions	syn2226551 ; syn2226432	Charlie Liu		Ashburn, Virginia, USA
CompModel-IGIB	syn1999433	Rintu Kutum	CSIR-Institute of Genomics & Integrative Biology	New Delhi, India
CQB	syn2226572	Dai Ziwei, Shao Bin	Center of Quantitative Biology, Peking University	Beijing, China
CytotoxicAvengers	syn2208220	Ravi Narasimhan		
D-Tox	syn2203318	Mathieu Clément-Ziza ^{1,2} , Michael Kuhn ¹ , Eleni G. Christodoulou ¹ , Susanne Reinhardt ¹ , and Andreas Beyer ^{1,2}	1 BIOTEC, Technical University of Dresden; 2 CECAD, University of Cologne	Dresden; Cologne, Germany
FastRun	syn2226802	Jungsoo Chang, Marianne Cowherd, Pelham Barron, and Inhan Lee	miRcore	Ann Arbor, Michigan, USA
FIN&al	syn2226548	Muhammad Ammad-uddin	Helsinki Institute for Information Technology, Department of Information and Computer Science, Aalto	Espoo, Finland

Team	Project	Team Members	Organization(s)	Location(s)
			University	
ICOS Team	syn2027319	Nicola Lazzarini, Dr. Jaume Bacardit	Newcastle University	Newcastle, UK
Kaiju	syn2196876	Michael K.K. Leung	University of Toronto	Toronto, Canada
mlcb	syn2227344	Chloé-Agathe Azencott, Karsten Borgwardt, Dominik Grimm, Felipe Llinares López, Carl Johann Simon-Gabriel	Machine Learning and Computational Biology Research Group, Max Planck Institutes for Developmental Biology and for Intelligent Systems	Tübingen, Germany
MPIMG	syn2227595	Matthias Heinig ^{1,2} , Matthew Huska ¹ , Alessandro Mammana ¹ , Alena van Bömmel ¹ , Juliane Perner ¹ , Brian Caffrey ¹ and Martin Vingron ¹	1 Max Planck Institute for molecular Genetics; 2 Max-Delbrück Center for Molecular Medicine	Berlin, Germany
O6d0A	syn2227297	Sean Whalen ^{1,2} , Gaurav Pandey ² , Douglas Ruderfer ²	1 Gladstone Institutes; 2 Mount Sinai	San Francisco; New York, USA
TeamRoslin	syn2223083 ; syn2226631	Konrad Rawlik, Sofie Demeyer, Tom Michoel, Albert Tenesa	Division of Genetics and Genomics, The Roslin Institute, University of Edinburgh	Scotland, UK
The fellowship of the ring	syn2223016 ; syn2223112	S. Alaimo ¹ , A. Pulvirenti ² , M. Mongioli ¹ , R. Giugno ² , R. Sharan ³ , A. Ferro ²	1 Department of Mathematics and Computer Science; 2 Department of Clinical and Molecular Biomedicine, University of Catania; 3 School of Computer Science, Tel-Aviv University	Catania, Italy; Tel-Aviv, Israel
UT_CCB	syn2227179	Liang-Chin Huang ¹ , Yonghui Wu ¹ , Yunguo Gong ¹ , Jeffrey Chang ^{1,2} , Trevor Cohen ¹ , Jingchun Sun ¹ , W. Jim Zheng ¹ , and Hua Xu ¹	1 School of Biomedical Informatics; 2 Department of Integrative Biology and Pharmacology, The University of Texas Health Science Center at Houston	Houston, Texas, USA

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WarwickDataScience	syn2211146	Richard S. Savage ^{1,2} , Jonathan D. Moore ¹	1 Systems Biology Centre; 2 Warwick Medical School, University of Warwick	Warwick, UK
Yang_Lab	syn2218909	Tao Wang, Hao Tang, Jichen Yang, Rui Zhong, Xiaowei Zhan, Yang Xie, Guanghua Xiao	University of Texas Southwestern Medical Center	Dallas, Texas, USA

Subchallenge 2

Team	Project	Team Members	Organization(s)	Location(s)
amss2012	syn376020	Junfei Zhao, Shihua Zhang	National Center for Mathematics and Interdisciplinary Sciences, Academy of Mathematics and Systems Science, Chinese Academy of Sciences	Beijing, China
Austria	syn2208373 ; syn2226984 ; syn2227016 ; syn2227023 ; syn2227030	Günter Klambauer, Andreas Mayr, and Sepp Hochreiter	Institute of Bioinformatics, Johannes Kepler University	Linz, Austria
Battelle Team	syn2223161	David A. Friedenber, Courtney A. Granville, Aaron J. Sander, Andrea L. Peabody, April M. Brys, Carol G. Riffle, Joel D. Elhard, Jenni W. Gorospe	Battelle	Columbus, Ohio, USA
borRf	syn2223113	Zofia Wiśniewska, Miron Bartosz Kurska	Interdisciplinary Centre for Mathematical and Computational Modelling, University of Warsaw	Warsaw, Poland
CompModel-IGIB	syn1999433	Rintu Kutum	CSIR-Institute of Genomics & Integrative Biology	New Delhi, India

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D-Tox	syn2203318	Michael Kuhn ¹ , Mathieu Clément-Ziza ^{1,2} , Susanne Reinhardt ¹ , and Andreas Beyer ^{1,2}	1 BIOTEC, Technical University of Dresden; 2 CECAD, University of Cologne	Dresden; Cologne, Germany
FIN&al	syn2226779	Muhammad Ammad-ud-din	Helsinki Institute for Information Technology, Department of Information and Computer Science, Aalto University	Espoo, Finland
ICOS Team	syn2331289	Nicola Lazzarini, Dr. Jaume Bacardit	Newcastle University	Newcastle, UK
Kaiju	syn2224382	Michael K.K. Leung	University of Toronto	Toronto, Canada
Lasige	syn2219104	Ana L. Teixeira ^{1,2} and Andre O. Falcao ¹	1 LaSIGE, Departamento de Informática, Faculdade de Ciências; 2 Centro de Química e Bioquímica, Faculdade de Ciências, Universidade de Lisboa	Lisboa, Portugal
mlcb	syn2226747	Chloé-Agathe Azencott, Karsten Borgwardt, Dominik Grimm, Felipe Llinares López, Carl Johann Simon-Gabriel	Machine Learning and Computational Biology Research Group, Max Planck Institutes for Developmental Biology and for Intelligent Systems	Tübingen, Germany
Opiyo	syn2226787	Stephen O. Opiyo	Molecular and Molecular Imaging Center, Ohio State University	Columbus, Ohio, USA
QBRC	syn2226486	Hao Tang, Jichen Yang, Tao Wang, Guanghua Xiao, Yang Xie	QBRC (Quantitative Biomedical Research Center), UT Southwestern Medical Center	Dallas, Texas, USA
Team Rocket	syn2180970	Weng Khong Lim	National Cancer Centre Singapore	Singapore