

2 - Supplementary Tables

Supplementary Table 1. Methods descriptions

Subchallenge 1	
rank	summary sentence
1	Kmeans clustering to divide cell lines into sub groups for prediction using randomForest
2	Kernel bilinear regression with an integrated cell lines kernel based on SNPs, RNA-Seq and covariates and a multi-task chemicals kernel based on empirical correlations.
3	Missing values were imputed, features were filtered based on their correlation to cytotoxicity data, random forests were trained for SNPs and RNAseq data, final predictions were the average of 2 individual models.
4	Used compound name and covariates to build a combined regression model
5	Kmeans clustering to divide cell lines into sub groups for prediction using randomForest
6	Averaged boosted trees / random forests on PLINK-preprocessed SNPs and EQTLs.
7	Kmeans clustering to divide cell lines into sub groups for prediction using randomForest
8	Systematic growth algorithm (SGA) is a novel polynomial time algorithm for learning nonlinear quantitative relationship from multiple input variables to single output.
9	Kmeans clustering to divide cell lines into sub groups for prediction using randomForest
10	Use compound name and covariates to build a combined regression model
11	A Random Forest model was learnt for each drug using the genotype data and the normalized RNA-seq data.
12	Kmeans clustering to divide cell lines into sub groups for prediction using randomForest
13	Kernel bilinear regression with a integrated cell lines kernel based on SNPs, RNA-Seq and covariates and a dirac chemicals kernel, with additional residuals boosting.
14	A multi-task learning approach using Random Forests, with SNP feature selection via fast GWAS, and bias correction for training/test set mismatch.
15	A neural network trained on selected SNPs and dimension-reduced chemical features to do regression on EC10 values
16	Systematic growth algorithm (SGA) is a novel polynomial time algorithm for learning nonlinear quantitative relationship from multiple input variables to single output.
19	Kernel bilinear regression with a linear cell lines kernel based on covariates and a slightly multitask chemicals kernel.
21	Missing SNPs were imputed, features were filtered based on their correlation to the cytotoxicity data, the generalized boosted regression models were trained for SNPs and RNA-seq respectively, the final predictions were obtained based on the average score from two individual models.
22	A multi-task learning approach using Random Forests, with SNP feature selection via fast GWAS, and bias correction for training/test set mismatch.
23	A multi-task learning approach using Random Forests, with SNP feature selection via fast GWAS, and bias correction for training/test set mismatch.
24	A multi-task learning approach using Random Forests, with SNP feature selection via fast GWAS, and bias correction for training/test set mismatch.
26	A multi-task learning approach using Random Forests, with SNP feature selection via fast GWAS, and bias correction for training/test set mismatch.
27	Missing SNPs were imputed, features were filtered based on their correlations to the cytotoxicity data, the elastic net models were trained for SNPs and RNA-seq data respectively, the final predictions were obtained based on the average score from two individual models.

28	Use compound name and covariates to build lasso regression
29	Multitask Gaussian Process with Tanimoto kernels.
31	The genomic data were combined with chemical descriptors to learn a single model simultaneously predicting the cytotoxicity of all drugs in all cell lines and the prediction were normalized.
32	Linear regression with supervised principal components is used to predict EC10 cytotoxicity with RNAseq and SNP data as predictors.
33	Phenotype specific AdaBoost ensemble of Regression Trees on covariates and SNPs selected by GWAS
34	One Random Forest model for each drug was learnt using only the genomic data as predictors.
35	We integrated a collection of machine-learning techniques and SNPs selection methods into a Bag-of-models-like approach where for each compound we selected the best performing method from the different combinations of machine-learning techniques and input features for prediction.
37	We integrated a collection of machine-learning techniques and SNPs selection methods into a Bag-of-models-like approach where for each compound we selected the best performing method from the different combinations of machine-learning techniques and input features for prediction.
38	Combination of Random Forest simultaneous prediction and drug by drug Random Forest model taking RNA-seq data into account.
39	The genomic data were combined with chemical descriptors to learn a single model simultaneously predicting the cytotoxicity of all drugs in all cell lines.
40	Predicting cellular toxicity with multiple layers of neural network.
41	Linear fitting of existing data.
42	The toxicity of an unknown cell was predicted by a weighted average of toxicity values of closely related cells, as defined by Pearson correlation coefficients of surrogate biomarkers for each toxin.
46	Kernel bilinear regression with a linear cell lines kernel based on covariates and a dirac chemicals kernel, with additional residuals boosting.
47	Linear fitting and using SNPs to get lower boundary of EC data.
48	Regularized least-squares regression with 10-fold cross-validation and elastic net on a selected set of genotypes, calculated with the Kruskal-Wallis test.
49	A machine learning approach that uses Feature Selection coupled with a regression method to resolve the problem of Toxicogenetic Dream Sub-Challenges.
50	The toxicity of an unknown cell was predicted by a weighted average of toxicity values of closely related cells, as defined by Pearson correlation coefficients of surrogate biomarkers for each toxin.
51	A machine learning approach that uses Feature Selection coupled with a regression method to resolve the problem of Toxicogenetic Dream Sub-Challenges.
52	Random forest predictions based on covariates, and Gram matrices for SNPs, RNA-Seq.
53	We have build continent specific models for each chemical cytotoxicity using random forest algorithm.
55	AdaBoost Ensemble of Regression Trees on selected SNPs and covariates
56	Gaussian process regression on a per-compound basis, tuning the set of SNPs used for each compound.
57	Linear regression with elastic net regression is used to predict EC10 cytotoxicity with RNAseq and SNP data as predictors.
58	An approach based on two dimensionality reduction techniques Locality-Sensitive Hashing (LSH) and Singular Value Decomposition (SVD) in connection to discriminative learning methods.
59	A machine learning approach that uses Feature Selection coupled with a regression method to resolve the problem of Toxicogenetic Dream Sub-Challenges.
61	Use compound name, covariates, RNA, and SNP to build a Lasso regression model

62	The toxicity of an unknown cell was predicted by a weighted average of toxicity values of closely related cells, as defined by Pearson correlation coefficients of surrogate biomarkers for each toxin.
63	Kernel based matrix factorization
66	A machine learning approach that uses Feature Selection coupled with a regression method to resolve the problem of Toxicogenetic Dream Sub-Challenges.
68	Linear regression with elastic net regression is used to predict EC10 cytotoxicity with RNAseq and SNP data as predictors.
69	Linear regression with elastic net regression is used to predict EC10 cytotoxicity with RNAseq and SNP data as predictors.
71	An approach based on two dimensionality reduction techniques Locality-Sensitive Hashing (LSH) and Singular Value Decomposition (SVD) in connection to discriminative learning methods.
72	Linear regression with elastic net regression is used to predict EC10 cytotoxicity with RNAseq and SNP data as predictors.
75	Gaussian process regression on a per-compound basis, tuning the set of SNPs used for each compound, and flipping the predictions of lowest quality.
76	Single task univariate linear regression over the first principal component computed on a reduced set of SNPs.
77	Bayesian Multiple Kernel Learning with additional input data
80	The toxicity of an unknown cell was predicted by a weighted average of toxicity values of closely related cells, as defined by Pearson correlation coefficients of surrogate biomarkers for each toxin.
82	The toxicity of an unknown cell was predicted by a weighted average of toxicity values of closely related cells, as defined by Pearson correlation coefficients of surrogate biomarkers for each toxin.
85	We estimate the probabilities of signal transduction for all the stimulus-response circuits of each signalling pathway from gene expression values, which are further used in a SVM \hat{a} -regression with k-fold cross-validation to obtain a prediction model.
86	Bayesian Multiple Kernel Learning
87	Predicting cellular toxicity with multiple layers of neural network.
89	Kernel based matrix factorization
90	Kernel based matrix factorization
91	Gaussian process regression on a per-compound basis.
92	this is only a random number generator.
93	Use compound name, covariates, RNA, and SNP to build an elastic-net regression model
94	A neural network trained on selected SNPs and dimension-reduced chemical features to do regression on EC10 values
95	Random forest regression using important SNP selection obtained by the Bourta method.
97	A neural network trained on selected SNPs and dimension-reduced chemical features to do regression on EC10 values
98	A neural network trained on selected SNPs and dimension-reduced chemical features to do regression on EC10 values
99	A neural network trained on selected SNPs and dimension-reduced chemical features to do regression on EC10 values

Subchallenge 2

rank	summary sentence
1	Our method used feature selection and group based models to predict cytotoxicities for new compounds.

2	Our method used group-based models for prediction.
3	We used group based models.
4	We used group based models.
5	We used group based models.
6	ElasticNet prediction of median and inter-quantile distance of log(EC10) as two independent problems
8	Random forest model with some simple variable selection beforehand
9	Molecules are characterized by biotechnological measurements (pharmacological analoging) rather than by their chemical structure (structural analoging).
10	Two kinds of feature: CDK and SiRMS were combined, generalized boosted regression model is constructed to do the prediction task.
11	Molecules are characterized by biotechnological measurements (pharmacological analoging) rather than by their chemical structure (structural analoging).
12	A hybrid approach using a selection method based on Random Forests to determine variable importance coupled with Support Vector Machines to model cytotoxicity to chemical compounds based on structural descriptors.
13	Molecules are characterized by biotechnological measurements (pharmacological analoging) rather than by their chemical structure (structural analoging).
14	A hybrid approach using a selection method based on Random Forests to determine variable importance coupled with Support Vector Machines to model populations median cytotoxicity to chemical compounds based on structural descriptors. Multivariate adaptive regression splines was applied to predict populations 5th and 95th cytotoxicity quartiles.
15	The set of chemical descriptors were expanded by using external sources and including metabolite information for the subsequent prediction of drug sensitivity with Random Forest.
16	Gradient Boosting Machine after simple variable selection step
17	Support vector regression prediction of median and inter-quantile distance of log(EC10) as two independent problems.
18	Greedy ensemble of several standard machine learning methods
19	Molecules are characterized by biotechnological measurements (pharmacological analoging) rather than by their chemical structure (structural analoging).
21	Two kinds of features were combined, the random forest model was trained to do the prediction task.
22	Molecules are characterized by biotechnological measurements (pharmacological analoging) rather than by their chemical structure (structural analoging).
24	The set of chemical descriptors were expanded by using external sources and including metabolite information for the subsequent prediction of drug sensitivity with Random Forest.
25	Ensemble prediction of median and inter-quantile distance of log(EC10) as two independent problems
26	A neural network trained on selected SNPs and dimension-reduced chemical features to do regression on EC10 values.
28	A neural network trained on selected SNPs and dimension-reduced chemical features to do regression on EC10 values.
29	A neural network trained on selected SNPs and dimension-reduced chemical features to do regression on EC10 values.
30	A neural network trained on selected SNPs and dimension-reduced chemical features to do regression on EC10 values.
31	Two kinds of features were combined, the principal component analysis technique was used to do dimension reduction, the linear regression model was trained to do the prediction task.
33	Kernel based matrix factorization
36	Two kinds of features were combined, the elastic net model was trained to do the prediction task.

37	A hybrid approach using a selection method based on Random Forests to determine variable importance coupled with Support Vector Machines to model cytotoxicity to chemical compounds based on structural descriptors.
38	We have used random forest (ensemble decision tree) algorithm to predict the cytotoxicity of chemicals using their chemical attributes.
40	Partial least squares (PLS) is a projection method where the independent variables, represented as the matrix X, are projected onto a low dimensional space. PLS uses both X and Y.
41	MARS (Multivariate Adaptive Regression Splines) model after simple preprocessing
42	A hybrid approach using a selection method based on Random Forests to determine variable importance coupled with Support Vector Machines to model populations median cytotoxicity to chemical compounds based on structural descriptors. Multivariate adaptive regression splines was applied to predict populations 5th and 95th cytotoxicity quartiles.
43	The set of chemical descriptors were expanded by using external sources and including metabolite information for the subsequent prediction of drug sensitivity with Random Forest.
46	Partial least squares (PLS) is a projection method where the independent variables, represented as the matrix X, are projected onto a low dimensional space. PLS uses both X and Y.
47	Kernel based matrix factorization
48	Partial least squares (PLS) is a projection method where the independent variables, represented as the matrix X, are projected onto a low dimensional space. PLS uses both X and Y.
49	Bayesian Multiple Kernel Learning with additional input data
50	A machine learning approach that uses Feature Selection coupled with a regression method to resolve the problem of Toxicogenetic Dream Sub-Challenges.
51	A hybrid approach using a selection method based on Random Forests to determine variable importance coupled with Support Vector Machines to model populations median cytotoxicity to chemical compounds based on structural descriptors. Multivariate adaptive regression splines was applied to predict populations 5th and 95th cytotoxicity quartiles.
52	Multi-task GP regression prediction of median and inter-quantile distance of log(EC10) as two independent problems.
54	An ensemble of 10 different machine learning models averaged together.
55	Partial least squares (PLS) is a projection method where the independent variables, represented as the matrix X, are projected onto a low dimensional space. PLS uses both X and Y.
58	Random Forest regression modelling EC10 from both important SNPs and chemical descriptors trained on a data from Subchallenge 1.
62	Kernel based matrix factorization
66	Kernel based matrix factorization
67	A neural network trained on selected SNPs and dimension-reduced chemical features to do regression on EC10 values.
74	k-nearest-neighbor prediction of median and inter-quantile distance of log(EC10) as two independent problems.
79	Partial least squares (PLS) is a projection method where the independent variables, represented as the matrix X, are projected onto a low dimensional space. PLS uses both X and Y.
80	Random Forest regression in R statistical environment was used to predict median values and interquartile ranges for EC10 in the 50 test compounds (for which no EC10 values were provided), based on a training dataset of 106 compounds.

[tables/SuppTable1aMethodsDescriptionsch1.pdf](#)
[tables/SuppTable1aMethodsDescriptionsch1.pdf](#)

Supplementary Table 2. 41 KEGG pathways, manually selected for dimension reduction

KEGG_ACUTE_MYELOID_LEUKEMIA	KEGG_NUCLEOTIDE_EXCISION_REPAIR
KEGG_APOPTOSIS	KEGG_P53_SIGNALING_PATHWAY
KEGG_BASAL_CELL_CARCINOMA	KEGG_PANCREATIC_CANCER
KEGG_BASAL_TRANSCRIPTION_FACTORS	KEGG_PATHWAYS_IN_CANCER
KEGG_BASE_EXCISION_REPAIR	KEGG_PEROXISOME
KEGG_BLADDER_CANCER	KEGG_PPAR_SIGNALING_PATHWAY
KEGG_CELL_CYCLE	KEGG_PROSTATE_CANCER
KEGG_CHRONIC_MYELOID_LEUKEMIA	KEGG_PROTEASOME
KEGG_CYTOKINE_CYTOKINE_RECEPTOR_INTERACTION	KEGG_REGULATION_OF_AUTOPHAGY
KEGG_DNA_REPLICATION	KEGG_RENAL_CELL_CARCINOMA
KEGG_ENDOMETRIAL_CANCER	KEGG_RNA_DEGRADATION
KEGG_ERBB_SIGNALING_PATHWAY	KEGG_RNA_POLYMERASE
KEGG_GLIOMA	KEGG_SMALL_CELL_LUNG_CANCER
KEGG_HOMOLOGOUS_RECOMBINATION	KEGG_SPLICEOSOME
KEGG_JAK_STAT_SIGNALING_PATHWAY	KEGG_TGF_BETA_SIGNALING_PATHWAY
KEGG_LYSOSOME	KEGG_THYROID_CANCER
KEGG_MAPK_SIGNALING_PATHWAY	KEGG_UBIQUITIN_MEDIATED_PROTEOLYSIS
KEGG_MELANOMA	KEGG_VEGF_SIGNALING_PATHWAY
KEGG_MISMATCH_REPAIR	KEGG_WNT_SIGNALING_PATHWAY
KEGG_MTOR_SIGNALING_PATHWAY	KEGG_NON_HOMOLOGOUS_END_JOINING
KEGG_NON_SMALL_CELL_LUNG_CANCER	

[tables/SuppTable2_KEGGpathways.pdf](#)

Supplementary Table 3. Chemical descriptors characterizing predictability

CDK descriptors	p
LipinskiFailures	0.016
BCUTp.1l	0.036

Dragon descriptors	p
MAXDP	0.038
MATS6m	0.028
MATS6v	0.030
MATS6p	0.040
GATS5m	0.026
GATS5v	0.009
GATS2e	0.025
GATS3p	0.029
GATS5p	0.041
JGI5	0.037
ALOGP	0.040
B02[C-O]	0.025
B04[C-C]	0.041

SIRMS descriptors	p
S_A.elm..C_H_H_O.1_2s.1_3s.1_4s.5	0.048
S_A.type..C.3_H_H_O.3.1_2s.1_3s.1_4s.5	0.048
Fr2.chg..C_D.1_2a.	0.041
Fr3.chg..A_C_D.1_3s.2_3a.	0.041
Fr3.chg..B_C_D.1_2a.2_3a.	0.041
S_A.chg..A_B_C_D.1_4s.2_3a.3_4a.6	0.041
S_A.chg..A_B_C_D.1_4s.3_4a.4	0.048
S_A.chg..B_C_C_D.1_2s.1_3a.3_4a.6	0.041
S_A.chg..B_C_D_D.1_2a.2_4a.4	0.049
Fr2.d_a..A_l.1_2s.	0.047

[tables/SuppTable3_ChemicalDescriptorsForPredictability.pdf](#)

Supplementary Table 4. Leaderboard subchallenge 1

team	rank PCI	mean PCI	max PCI	mean ranking PCI	z-score mean ranking PCI	FDR mean ranking PCI	rank PC	mean PC	max PC	mean ranking PC	z-score mean ranking PC	FDR mean ranking PC	mean ranking	rank
Yang_Lab	1	0.514	0.553	27.22	-7.60	0.00	2	0.053	0.233	31.87	-6.05	0.00	1.5	1
CASSIS	2	0.512	0.557	31.57	-6.15	0.00	4	0.048	0.215	34.35	-5.22	0.00	3	2
amss2012	3	0.511	0.552	34.81	-5.07	0.00	5	0.045	0.205	36.67	-4.45	0.00	4	3
UT_CCB	11	0.510	0.563	38.82	-3.73	0.00	1	0.068	0.279	28.15	-7.29	0.00	6	4
Yang_Lab	4	0.510	0.554	36.05	-4.65	0.00	10	0.043	0.231	38.01	-4.00	0.00	7	5.5
O6d0A	6	0.510	0.545	36.35	-4.55	0.00	8	0.043	0.186	37.89	-4.04	0.00	7	5.5
Yang_Lab	8	0.510	0.553	37.93	-4.03	0.00	7	0.041	0.207	37.77	-4.08	0.00	7.5	7
CQB	7	0.510	0.552	37.21	-4.27	0.00	9	0.046	0.220	37.93	-4.03	0.00	8	8
Yang_Lab	5	0.510	0.552	36.27	-4.58	0.00	13	0.039	0.204	40.07	-3.31	0.00	9	9.5
UT_CCB	15	0.508	0.543	41.07	-2.98	0.01	3	0.050	0.194	32.81	-5.73	0.00	9	9.5
D-Tox	13	0.510	0.545	39.05	-3.65	0.00	6	0.044	0.279	37.35	-4.22	0.00	9.5	11
Yang_Lab	10	0.509	0.557	38.81	-3.73	0.00	11	0.041	0.221	38.19	-3.94	0.00	10.5	12
CASSIS	9	0.510	0.552	38.29	-3.91	0.00	15	0.038	0.212	40.20	-3.27	0.00	12	13
WarwickDataScience	12	0.509	0.545	38.90	-3.70	0.00	14	0.035	0.187	40.15	-3.29	0.00	13	14
Kaiju	14	0.508	0.541	40.31	-3.23	0.00	16	0.032	0.201	41.44	-2.86	0.01	15	15.5
CQB	18	0.508	0.541	43.14	-2.29	0.06	12	0.041	0.170	38.33	-3.89	0.00	15	15.5
UTSW_QBRC	16	0.508	0.551	42.24	-2.59	0.03	17	0.031	0.215	42.47	-2.51	0.03	16.5	17
QBRC_UTSW_km48	17	0.507	0.549	42.51	-2.50	0.04	20	0.027	0.212	44.37	-1.88	0.15	18.5	18
CASSIS	22	0.507	0.552	44.33	-1.89	0.13	18	0.032	0.226	43.74	-2.09	0.10	20	19
UTSW_QBRC_km36	19	0.507	0.549	43.35	-2.22	0.07	24	0.026	0.212	45.00	-1.67	0.20	21.5	20
amss2012	25	0.507	0.550	45.11	-1.63	0.20	19	0.031	0.185	44.13	-1.96	0.13	22	21
WarwickDataScience	21	0.507	0.540	43.92	-2.03	0.10	25	0.028	0.180	45.10	-1.64	0.20	23	23
WarwickDataScience	23	0.507	0.542	44.54	-1.82	0.15	23	0.028	0.185	44.96	-1.68	0.20	23	23
WarwickDataScience	24	0.507	0.544	44.70	-1.77	0.16	22	0.027	0.171	44.76	-1.75	0.18	23	23
NEXUS	29	0.506	0.544	45.55	-1.48	0.23	21	0.028	0.195	44.42	-1.86	0.15	25	25
WarwickDataScience	20	0.507	0.542	43.71	-2.10	0.09	32	0.026	0.185	46.19	-1.27	0.31	26	26
amss2012	26	0.506	0.539	45.25	-1.58	0.21	27	0.027	0.187	45.37	-1.54	0.22	26.5	27
UT_CCB	28	0.506	0.542	45.48	-1.51	0.23	26	0.026	0.171	45.11	-1.63	0.20	27	28
mlcb	27	0.506	0.539	45.27	-1.58	0.21	31	0.024	0.175	46.02	-1.33	0.29	29	29
YODAsttest	30.5	0.506	0.545	45.65	-1.45	0.23	28	0.026	0.198	45.51	-1.50	0.23	29.25	30
D-Tox	32	0.507	0.545	45.73	-1.43	0.24	35	0.027	0.220	46.57	-1.14	0.35	33.5	31
CytotoxicAvengers	37	0.506	0.536	46.67	-1.11	0.36	33	0.024	0.159	46.26	-1.25	0.32	35	32.5
TeamRoslin	40	0.505	0.535	47.99	-0.67	0.62	30	0.027	0.185	45.64	-1.45	0.24	35	32.5
D-Tox	30.5	0.507	0.545	45.65	-1.45	0.23	40	0.027	0.224	47.22	-0.93	0.44	35.25	34
MPIMG	43	0.505	0.551	48.38	-0.54	0.66	29	0.026	0.215	45.52	-1.50	0.23	36	35
UTSW_QBRC	35	0.506	0.553	46.62	-1.13	0.36	38	0.022	0.215	46.66	-1.11	0.35	36.5	36
MPIMG	38	0.505	0.552	47.37	-0.88	0.49	36	0.023	0.215	46.63	-1.13	0.35	37	37
D-Tox	34	0.506	0.542	46.12	-1.29	0.28	43	0.024	0.190	47.64	-0.79	0.50	38.5	38

D-Tox	33	0.506	0.539	45.88	-1.37	0.25	45	0.021	0.183	48.13	-0.62	0.59	39	39.5
Charlie's Minions	39	0.505	0.534	47.84	-0.72	0.60	39	0.021	0.140	47.09	-0.97	0.42	39	39.5
CQB	42	0.505	0.550	48.23	-0.59	0.65	37	0.029	0.160	46.64	-1.12	0.35	39.5	41
FastRun	36	0.505	0.531	46.64	-1.12	0.36	46	0.017	0.144	48.44	-0.52	0.65	41	42
PNNL	44	0.505	0.552	48.38	-0.54	0.66	42	0.023	0.190	47.41	-0.87	0.46	43	43
Battelle Team	41	0.506	0.551	48.13	-0.62	0.64	48	0.023	0.211	49.15	-0.28	0.79	44.5	44
YODAsttest	51	0.505	0.548	50.40	0.13	1.00	41	0.024	0.194	47.35	-0.88	0.46	46	45
CASSIS	46	0.505	0.552	48.96	-0.35	0.78	49	0.020	0.202	49.19	-0.27	0.79	47.5	46.5
CQB	61	0.503	0.541	51.77	0.59	1.00	34	0.024	0.143	46.52	-1.16	0.35	47.5	46.5
TeamRoslin	45	0.505	0.538	48.44	-0.52	0.66	53	0.018	0.170	49.84	-0.05	0.89	49	48
ICOS Team	55	0.504	0.542	51.03	0.34	1.00	44	0.024	0.203	48.10	-0.63	0.59	49.5	49
FastRun	47	0.504	0.536	49.60	-0.13	0.94	54	0.014	0.143	50.23	0.08	0.97	50.5	50
ICOS Team	56	0.504	0.539	51.07	0.36	1.00	47	0.023	0.199	48.51	-0.50	0.65	51.5	51
CASSIS	48	0.505	0.547	49.70	-0.10	0.94	56	0.017	0.182	50.71	0.24	1.00	52	52
CompModel-IGIB	50	0.504	0.538	49.88	-0.04	0.96	58	0.014	0.155	51.14	0.38	1.00	54	53
CompModel-IGIB	52	0.504	0.539	50.62	0.21	1.00	59	0.015	0.119	51.25	0.42	1.00	55.5	54
TeamRoslin	64	0.504	0.542	52.52	0.84	1.00	50	0.019	0.171	49.36	-0.21	0.82	57	55.5
mlcb	53	0.504	0.539	50.82	0.27	1.00	61	0.014	0.175	51.75	0.58	1.00	57	55.5
CytotoxicAvengers	63	0.503	0.532	52.02	0.67	1.00	52	0.016	0.155	49.46	-0.18	0.82	57.5	57.5
The fellowship of the ring	60	0.504	0.541	51.66	0.55	1.00	55	0.016	0.190	50.47	0.16	1.00	57.5	57.5
ICOS Team	59	0.504	0.538	51.56	0.52	1.00	57	0.018	0.265	51.09	0.36	1.00	58	60
Purdue Xie	49	0.504	0.534	49.73	-0.09	0.94	67	0.009	0.129	52.74	0.91	1.00	58	60
UT_CCB	65	0.502	0.536	52.87	0.96	1.00	51	0.016	0.165	49.43	-0.19	0.82	58	60
FastRun	54	0.503	0.532	50.92	0.31	1.00	63	0.009	0.158	51.92	0.64	1.00	58.5	62
FIN&al	57	0.503	0.539	51.23	0.41	1.00	69	0.006	0.155	53.54	1.18	1.00	63	63
CompModel-IGIB	62	0.503	0.534	51.85	0.62	1.00	65	0.013	0.162	52.18	0.73	1.00	63.5	64
UTSW_QBRC_km45	58	0.504	0.547	51.26	0.42	1.00	72	0.013	0.194	53.89	1.30	1.00	65	65.5
ICOS Team	70	0.502	0.541	54.75	1.58	1.00	60	0.016	0.193	51.64	0.55	1.00	65	65.5
CompModel-IGIB	67	0.503	0.536	53.56	1.19	1.00	64	0.014	0.163	52.05	0.69	1.00	65.5	67
CytotoxicAvengers	69	0.502	0.536	54.46	1.49	1.00	66	0.007	0.153	52.27	0.76	1.00	67.5	68
CytotoxicAvengers	71	0.502	0.540	54.99	1.66	1.00	68	0.007	0.150	53.27	1.09	1.00	69.5	69.5
CompModel-IGIB	66	0.503	0.534	53.14	1.05	1.00	73	0.009	0.159	54.07	1.36	1.00	69.5	69.5
The fellowship of the ring	73	0.503	0.541	55.09	1.70	1.00	70	0.013	0.178	53.56	1.19	1.00	71.5	71
CytotoxicAvengers	74	0.501	0.536	55.30	1.77	1.00	71	0.006	0.154	53.64	1.21	1.00	72.5	72
sshh	72	0.502	0.532	55.05	1.69	1.00	74	0.009	0.150	54.24	1.42	1.00	73	73
TeamDaniel	86	0.500	0.529	59.43	3.15	1.00	62	0.013	0.136	51.76	0.59	1.00	74	74
mlcb	75	0.502	0.538	56.21	2.07	1.00	76	0.003	0.151	55.59	1.87	1.00	75.5	75.5
mlcb	76	0.501	0.534	56.40	2.13	1.00	75	0.007	0.146	54.69	1.57	1.00	75.5	75.5
FIN&al	79	0.501	0.534	57.27	2.43	1.00	78	0.005	0.138	56.52	2.17	1.00	78.5	77
RNlgroup	78	0.500	0.543	57.18	2.39	1.00	83	-0.001	0.144	57.32	2.44	1.00	80.5	78.5
PNNL	82	0.500	0.536	58.75	2.92	1.00	79	0.003	0.145	56.57	2.19	1.00	80.5	78.5

FastRun	77	0.500	0.528	57.02	2.34	1.00	86	-0.003	0.132	57.96	2.65	1.00	81.5	80.5
PNNL	83	0.500	0.538	59.05	3.02	1.00	80	0.003	0.142	56.60	2.20	1.00	81.5	80.5
FastRun	80	0.500	0.531	57.46	2.49	1.00	84	-0.003	0.162	57.40	2.47	1.00	82	82.5
PNNL	87	0.500	0.532	59.60	3.20	1.00	77	0.003	0.155	56.48	2.16	1.00	82	82.5
PNNL	84	0.500	0.537	59.10	3.04	1.00	81	0.003	0.143	56.75	2.25	1.00	82.5	84
bioinfoCIPF	68	0.501	0.533	54.27	1.43	1.00	99	NA	NA	98.93	16.33	1.00	83.5	85
FIN&al	81	0.501	0.531	58.31	2.77	1.00	88	0.000	0.151	59.46	3.16	1.00	84.5	86
Charlie's Minions	85	0.499	0.533	59.32	3.11	1.00	85	-0.002	0.152	57.91	2.64	1.00	85	87
TeamDaniel	89	0.499	0.524	60.27	3.43	1.00	82	0.000	0.104	56.99	2.33	1.00	85.5	88
FIN&al	88	0.500	0.539	59.95	3.32	1.00	90	-0.003	0.147	59.76	3.26	1.00	89	89.5
FIN&al	91	0.499	0.529	61.09	3.70	1.00	87	0.000	0.168	58.23	2.75	1.00	89	89.5
mlcb	90	0.499	0.554	60.89	3.63	1.00	89	-0.007	0.212	59.52	3.18	1.00	89.5	91
CQB	92	0.498	0.538	61.88	3.96	1.00	92	-0.009	0.146	60.93	3.65	1.00	92	92
UT_CCB	94	0.498	0.528	62.76	4.26	1.00	91	-0.006	0.122	59.87	3.29	1.00	92.5	93
Kaiju	93	0.498	0.525	62.49	4.17	1.00	95	-0.019	0.114	66.79	5.60	1.00	94	94
BorRfLm	96	0.499	0.537	64.65	4.89	1.00	93	-0.007	0.152	63.22	4.41	1.00	94.5	95.5
PCM	95	0.498	0.520	62.96	4.32	1.00	94	-0.014	0.097	63.53	4.51	1.00	94.5	95.5
Kaiju	97	0.496	0.525	66.41	5.47	1.00	97	-0.023	0.119	68.64	6.22	1.00	97	97
Kaiju	99	0.496	0.526	68.43	6.15	1.00	96	-0.023	0.117	68.63	6.21	1.00	97.5	98
Kaiju	98	0.496	0.524	67.56	5.86	1.00	98	-0.023	0.116	69.23	6.42	1.00	98	99

[tables/SuppTable4Leaderboardfinal_sch1.pdf](#)

Supplementary Table 5. Leaderboard subchallenge 2

team	mean ranking PC	rank PC	PC _m	PC _m pval	PC _q	PC _q pval	PC Fisher pval	PC Fisher FDR	mean ranking SC	rank SC	SC _m	SC _m pval	SC _q	SC _q pval	SC Fisher pval	SC Fisher FDR	mean ranking	rank
QBRC	7	1	0.52	0.00	0.37	0.00	0.00	0.00	9	2	0.45	0.00	0.40	0.00	0.00	0.00	1.5	1.5
QBRC	9	2	0.52	0.00	0.31	0.01	0.00	0.00	7	1	0.45	0.00	0.48	0.00	0.00	0.00	1.5	1.5
QBRC	9	3	0.44	0.00	0.34	0.01	0.00	0.00	10	3	0.43	0.00	0.45	0.00	0.00	0.00	3.0	3.0
QBRC	10	4	0.43	0.00	0.34	0.01	0.00	0.00	11	4	0.41	0.00	0.45	0.00	0.00	0.00	4.0	4.0
QBRC	18	7	0.44	0.00	0.19	0.09	0.00	0.00	12	6	0.42	0.00	0.38	0.00	0.00	0.00	6.5	5.0
mlcb	19	10	0.32	0.01	0.28	0.03	0.00	0.01	25	10	0.32	0.01	0.31	0.02	0.00	0.01	9.5	6.0
newDream	20	12	0.56	0.00	0.13	0.18	0.00	0.00	21	8	0.34	0.01	0.34	0.01	0.00	0.00	10.0	7.0
Battelle Team	26	18	0.34	0.01	0.15	0.16	0.01	0.03	21	7	0.36	0.01	0.33	0.01	0.00	0.00	12.5	8.0
Austria	13	6	0.65	0.00	0.15	0.15	0.00	0.00	32	20	0.72	0.00	0.03	0.43	0.00	0.00	12.8	9.5
austria	13	6	0.65	0.00	0.15	0.15	0.00	0.00	32	20	0.72	0.00	0.03	0.43	0.00	0.00	12.8	9.5
amss2012	24	17	0.27	0.03	0.26	0.03	0.01	0.03	25	12	0.25	0.04	0.38	0.00	0.00	0.01	14.3	11.0
Austria	19	10	0.65	0.00	0.12	0.20	0.00	0.00	32	20	0.70	0.00	0.04	0.40	0.00	0.00	14.8	12.0
Lasige	22	15	0.35	0.01	0.15	0.15	0.01	0.03	30	16	0.37	0.00	0.16	0.13	0.00	0.01	15.3	13.0
Austria	19	10	0.65	0.00	0.12	0.21	0.00	0.00	34	25	0.72	0.00	0.01	0.47	0.00	0.00	17.3	14.5
austria	19	10	0.65	0.00	0.12	0.21	0.00	0.00	34	25	0.72	0.00	0.01	0.47	0.00	0.00	17.3	14.5
Lasige	21	14	0.40	0.00	0.17	0.11	0.00	0.01	33	22	0.38	0.00	0.10	0.25	0.01	0.02	18.0	16.0
D-Tox	27	20	0.64	0.00	0.09	0.26	0.00	0.00	30	17	0.65	0.00	0.07	0.31	0.00	0.00	18.5	17.5
Battelle Team	32	24	0.30	0.02	0.12	0.20	0.02	0.07	27	13	0.36	0.01	0.22	0.06	0.00	0.01	18.5	17.5
mlcb	37	34	0.30	0.02	0.10	0.24	0.03	0.07	12	5	0.45	0.00	0.36	0.00	0.00	0.00	19.3	19.0
Battelle Team	36	31	0.41	0.00	0.06	0.34	0.00	0.02	25	12	0.41	0.00	0.18	0.10	0.00	0.01	21.0	20.0
Austria	20	13	0.66	0.00	0.11	0.22	0.00	0.00	38	35	0.69	0.00	0.00	0.51	0.00	0.00	23.8	21.0
newDream	36	31	0.12	0.21	0.20	0.08	0.08	0.15	32	18	0.12	0.20	0.45	0.00	0.00	0.01	24.3	22.0
amss2012	39	36	0.31	0.01	0.07	0.32	0.03	0.08	29	14	0.34	0.01	0.23	0.05	0.00	0.01	24.8	23.5
Austria	26	19	0.65	0.00	0.09	0.27	0.00	0.00	36	31	0.72	0.00	0.01	0.47	0.00	0.00	24.8	23.5
TeamDaniel	35	29	0.10	0.24	0.24	0.05	0.06	0.13	34	23	0.13	0.19	0.35	0.01	0.01	0.03	25.8	25.0
D-Tox	35	27	0.64	0.00	-0.02	0.56	0.00	0.00	35	27	0.65	0.00	0.03	0.42	0.00	0.00	27.0	26.5
mlcb	44	45	0.28	0.03	0.04	0.40	0.06	0.13	25	10	0.40	0.00	0.19	0.09	0.00	0.01	27.0	26.5
Kaiju	31	22	0.13	0.19	0.28	0.02	0.03	0.08	38	36	0.16	0.13	0.24	0.05	0.04	0.07	29.0	28.5
Experimental	44	43	0.17	0.12	0.11	0.23	0.12	0.20	30	16	0.36	0.00	0.17	0.12	0.00	0.01	29.0	28.5
Kaiju	32	26	0.10	0.24	0.29	0.02	0.03	0.08	37	33	0.18	0.10	0.24	0.05	0.03	0.06	29.3	30.0
Kaiju	28	21	0.13	0.19	0.31	0.02	0.02	0.06	39	39	0.16	0.13	0.24	0.05	0.04	0.07	29.8	31.0
Kaiju	31	23	0.14	0.16	0.23	0.05	0.05	0.10	38	37	0.19	0.09	0.23	0.05	0.03	0.06	30.0	32.0
amss2012	23	16	0.26	0.03	0.28	0.02	0.01	0.02	47	51	0.05	0.37	0.26	0.04	0.07	0.10	33.5	33.5

TeamPal	35	29	0.12	0.21	0.22	0.06	0.07	0.14	39	39	0.10	0.25	0.30	0.02	0.03	0.06	33.5	33.5
FIN&al	41	38	0.30	0.02	0.07	0.32	0.03	0.08	36	31	0.33	0.01	0.14	0.17	0.01	0.03	34.0	35.0
Experimental	43	41	0.24	0.05	0.08	0.30	0.07	0.14	35	29	0.30	0.02	0.18	0.11	0.01	0.03	35.0	36.0
Experimental	47	50	0.14	0.17	0.10	0.24	0.17	0.26	34	25	0.32	0.01	0.18	0.11	0.01	0.03	37.5	37.0
amss2012	45	48	0.19	0.09	0.08	0.30	0.12	0.20	35	28	0.36	0.01	0.10	0.25	0.01	0.03	38.0	38.0
Lasige	43	39	0.35	0.01	-0.03	0.58	0.02	0.07	41	41	0.33	0.01	0.08	0.30	0.02	0.04	40.0	39.0
CompModel-IGIB	45	47	0.17	0.12	0.10	0.24	0.13	0.20	38	35	0.25	0.04	0.19	0.10	0.03	0.05	40.5	40.0
Experimental	47	50	0.28	0.03	-0.01	0.52	0.07	0.14	37	32	0.34	0.01	0.09	0.26	0.01	0.03	41.0	41.0
Opiyo	32	26	0.18	0.11	0.16	0.14	0.08	0.15	52	58	0.09	0.26	0.12	0.21	0.21	0.26	41.5	42.0
Battelle Team	37	34	0.43	0.00	0.00	0.51	0.00	0.02	47	53	0.26	0.03	0.06	0.34	0.06	0.09	43.3	43.5
Lasige	41	38	0.55	0.00	-0.07	0.69	0.00	0.00	44	49	0.51	0.00	-0.04	0.62	0.00	0.00	43.3	43.5
D-Tox	45	47	0.64	0.00	-0.11	0.78	0.00	0.00	42	43	0.65	0.00	-0.02	0.56	0.00	0.00	44.5	45.0
Experimental	49	53	0.24	0.05	-0.01	0.53	0.11	0.19	40	40	0.30	0.02	0.10	0.24	0.03	0.06	46.5	46.0
UT_CCB	39	36	0.09	0.27	0.20	0.08	0.10	0.17	53	61	0.13	0.18	0.08	0.30	0.21	0.26	48.0	47.0
Opiyo	36	32	0.12	0.21	0.20	0.09	0.09	0.16	55	65	0.01	0.47	0.15	0.15	0.26	0.31	48.5	48.0
FIN&al	47	52	0.29	0.02	-0.02	0.55	0.07	0.14	43	46	0.31	0.01	0.08	0.29	0.03	0.06	49.0	49.0
Opiyo	44	43	0.03	0.42	0.21	0.07	0.13	0.20	52	58	-0.02	0.55	0.23	0.05	0.13	0.17	50.0	50.0
FIN&al	51	60	0.34	0.01	-0.09	0.73	0.04	0.08	42	43	0.37	0.00	0.03	0.42	0.01	0.03	51.3	51.0
ICOS Team	50	57	0.09	0.27	0.11	0.22	0.23	0.31	43	46	0.08	0.29	0.27	0.03	0.05	0.07	51.5	53.5
ICOS Team	50	57	0.09	0.27	0.11	0.22	0.23	0.31	43	46	0.08	0.29	0.27	0.03	0.05	0.07	51.5	53.5
ICOS Team	50	57	0.09	0.27	0.11	0.22	0.23	0.31	43	46	0.08	0.29	0.27	0.03	0.05	0.07	51.5	53.5
ICOS Team	50	57	0.09	0.27	0.11	0.22	0.23	0.31	43	46	0.08	0.29	0.27	0.03	0.05	0.07	51.5	53.5
Lasige	44	45	0.35	0.01	-0.05	0.64	0.03	0.08	54	62	0.37	0.00	-0.14	0.83	0.02	0.05	53.3	56.0
mlcb	50	57	0.46	0.00	-0.22	0.94	0.00	0.01	48	54	0.57	0.00	-0.13	0.81	0.00	0.00	55.5	57.0
newDream	55	63	-0.15	0.84	0.13	0.18	0.44	0.54	46	50	-0.09	0.74	0.34	0.01	0.04	0.07	56.5	58.0
Battelle Team	43	40	-0.09	0.74	0.29	0.02	0.08	0.15	63	74	-0.03	0.59	0.08	0.29	0.47	0.51	57.0	59.0
Opiyo	47	50	0.12	0.20	0.11	0.22	0.18	0.27	56	68	0.12	0.19	0.07	0.32	0.23	0.29	59.0	60.5
newDream	57	66	-0.31	0.99	0.13	0.18	0.48	0.56	47	52	-0.09	0.74	0.34	0.01	0.04	0.07	59.0	60.5
newDream	56	64	-0.23	0.95	0.13	0.18	0.47	0.55	48	55	-0.29	0.98	0.34	0.01	0.05	0.07	59.5	62.0
borRf	50	54	0.33	0.01	-0.08	0.72	0.04	0.10	56	66	0.32	0.01	-0.03	0.59	0.04	0.07	60.0	63.0
ssh	58	68	0.29	0.02	-0.17	0.87	0.08	0.15	51	56	0.24	0.04	0.06	0.35	0.08	0.12	62.0	64.0
RNIgroup	52	61	-0.02	0.57	0.15	0.16	0.30	0.40	56	68	0.05	0.38	0.13	0.19	0.26	0.31	64.5	65.0
CompModel-IGIB	63	72	0.10	0.26	-0.05	0.64	0.46	0.55	53	59	0.23	0.06	0.05	0.35	0.10	0.14	65.3	67.0
FIN&al	58	67	0.23	0.06	-0.09	0.73	0.17	0.26	55	64	0.27	0.03	-0.01	0.53	0.08	0.11	65.3	67.0

UT_CCB	61	70	0.07	0.32	-0.03	0.41	0.39	0.50	53	61	0.23	0.05	0.03	0.41	0.10	0.14	65.3	67.0
UT_CCB	60	69	0.16	0.13	-0.08	0.70	0.31	0.40	55	64	0.26	0.04	0.00	0.50	0.09	0.13	66.3	69.0
UT_CCB	57	65	0.17	0.11	-0.06	0.66	0.27	0.36	61	72	0.26	0.04	-0.05	0.63	0.11	0.15	68.5	70.0
FIN&al	55	62	0.17	0.11	-0.06	0.66	0.27	0.36	65	77	0.23	0.05	-0.06	0.65	0.15	0.20	69.3	71.0
Kaiju	63	72	0.04	0.39	0.03	0.43	0.46	0.55	56	68	0.06	0.34	0.10	0.24	0.29	0.33	69.8	72.0
CompModel-IGIB	67	75	-0.02	0.55	-0.01	0.52	0.64	0.70	58	71	0.13	0.19	0.04	0.39	0.27	0.32	73.0	73.0
TeamPal	71	77	0.02	0.43	-0.07	0.68	0.66	0.71	57	70	0.01	0.48	0.14	0.17	0.28	0.33	73.5	74.5
RNIgroup	67	74	0.05	0.36	-0.04	0.60	0.55	0.63	62	73	0.06	0.33	0.06	0.34	0.36	0.39	73.5	74.5
UT_CCB	63	73	0.10	0.25	-0.06	0.66	0.46	0.55	65	77	0.22	0.06	-0.05	0.64	0.16	0.21	74.8	76.0
TeamPal	75	80	0.00	0.51	-0.09	0.72	0.74	0.77	63	75	-0.08	0.71	0.09	0.26	0.50	0.53	77.5	77.0
CompModel-IGIB	74	79	0.08	0.30	-0.11	0.79	0.58	0.66	68	78	0.15	0.15	-0.05	0.64	0.32	0.36	78.3	78.0
mlcb	74	79	0.08	0.30	-0.14	0.84	0.60	0.67	71	80	0.06	0.33	-0.01	0.53	0.49	0.52	79.3	79.0
Kalpesh Shelke	68	76	-0.09	0.73	0.00	0.51	0.74	0.77	78	84	-0.11	0.77	-0.02	0.54	0.78	0.79	80.0	80.0
CompModel-IGIB	75	82	0.07	0.31	-0.15	0.84	0.61	0.67	69	79	0.16	0.14	-0.08	0.72	0.33	0.37	80.3	81.0
TeamDaniel	75	82	0.02	0.44	-0.09	0.74	0.69	0.73	75	83	0.01	0.48	-0.03	0.57	0.63	0.65	82.0	82.0
WarwickDataScience	80	84	0.01	0.46	-0.17	0.89	0.78	0.79	73	81	0.09	0.27	-0.08	0.71	0.51	0.53	82.5	83.0
Opiyo	79	83	-0.13	0.81	-0.10	0.76	0.91	0.92	75	83	-0.04	0.60	-0.01	0.53	0.68	0.70	82.8	84.0
Team Rocket	81	85	-0.23	0.95	-0.10	0.76	0.96	0.96	81	85	-0.26	0.97	-0.04	0.62	0.91	0.91	85.0	85.0

tables/SuppTable5Leaderboardfinal_sch2.pdf

Supplementary Table 6. Additional data and methods used

Subchallenge 1	
other input data	
KEGG pathway	
EQTLs	
known drug targets	
chemicals fingerprints	
BioAssay data	
predicted toxicity data	
Drug2Gene database (http://www.drug2gene.com)	
Connectivity Map (Lamb 2006)	
GO toxicity terms	
additional 1d,2d&3d attributes	
signaling pathways	
genesets summaries	
paradigm pathways summaries	
SNP mapped gene sets summaries	
Population types	
other dimension reduction	
use the gene expression as an intermediate featur	
Locality-Sensitive Hashing and Singular Value Decomposition	
other prediction algorithm	
Systematic growth algorithm	
Neural network	
Conditional Inference Trees	
Random Number Generator	
other model validation	
repeated random sub-sampling validation	
bootstrapping	
4-fold cross validation: 3 folds for training, 1 fold for validation	
computing best γ and cost parameters among different values tested	

Subchallenge 2	
other input data	
Chemical attributes (Dragon)	
ChEMBL	
PubChem	
Binary Fingerprints	
chemicals fingerprints	
BioAssay data	
predicted toxicity data	
ECP chemical descriptors, based on the SDF files provided.	
additional 1d, 2d&3d chemical attributes	
SNP mapped gene sets summaries	
Population types	
Pentacles	
Volsurf	
PubChem Fingerprints	
Maccs Fingerprints	
1D&2D physio-chemical descriptors	
Population effects	
other dimension reduction	
use the gene expression as an intermediate featur	
Locality-Sensitive Hashing and Singular Value Decomposition	
other prediction algorithm	
remove descriptors with high pair wise correlation	
other prediction algorithm	
Pharmacological Analoging	
Neural network	
nearest neighbors	
other model validation	
repeated random sub-sampling validation	
bootstrapping	
2-fold cross-validation	
4-fold cross validation: 3 folds for training, 1 fold for validation	

tables/SuppTable6_additionalMethodsData.pdf

Supplementary Table 7. Scores subchallenge 1 considering all 106 compounds

team	mean PC	max PC	mean ranking PC	rank PC	mean PCI	max PCI	mean ranking PCI	rank PCI
Yang_Lab	0.05	0.23	34.40	3	0.51	0.55	30.42	1
UT_CCB	0.07	0.28	28.01	1	0.51	0.56	35.83	4
CASSIS	0.04	0.22	36.12	4	0.51	0.56	33.32	2
amss2012	0.04	0.21	37.47	5	0.51	0.55	35.78	3
O6d0A	0.04	0.19	38.73	7	0.51	0.55	37.37	5
Yang_Lab	0.04	0.23	39.68	10	0.51	0.55	38.14	6
UT_CCB	0.05	0.19	33.19	2	0.51	0.54	40.69	14
Yang_Lab	0.04	0.21	38.83	8	0.51	0.55	38.55	9
D-Tox	0.04	0.28	38.67	6	0.51	0.55	39.82	13
CQB	0.04	0.22	39.90	11	0.51	0.55	38.53	8
Yang_Lab	0.04	0.22	38.93	9	0.51	0.56	39.29	11
WarwickDataScience	0.03	0.19	40.27	12	0.51	0.55	38.97	10
Yang_Lab	0.03	0.20	41.44	15	0.51	0.55	38.27	7
CASSIS	0.03	0.21	41.42	14	0.51	0.55	39.59	12
Kaiju	0.03	0.20	42.26	16	0.51	0.54	41.69	15
CQB	0.03	0.17	40.42	13	0.51	0.54	43.85	20
WarwickDataScience	0.03	0.18	44.05	18	0.51	0.54	43.11	16
UTSW_QBRC	0.03	0.22	42.96	17	0.51	0.55	44.28	21
WarwickDataScience	0.03	0.19	44.31	20	0.51	0.54	43.32	18
CASSIS	0.03	0.23	44.21	19	0.51	0.55	44.60	22
QBRC_UTSW_km48	0.02	0.21	45.14	23	0.51	0.55	43.81	19
amss2012	0.03	0.19	44.36	22	0.51	0.55	44.72	23
WarwickDataScience	0.03	0.19	45.69	29	0.51	0.54	43.26	17
UT_CCB	0.02	0.17	44.35	21	0.51	0.54	44.97	26
WarwickDataScience	0.03	0.17	45.17	24	0.51	0.54	45.10	29
UTSW_QBRC_km36	0.02	0.21	45.68	28	0.51	0.55	44.98	27
MPIMG	0.02	0.22	45.46	25	0.51	0.55	45.31	30
D-Tox	0.03	0.22	46.09	32	0.51	0.55	44.87	24
D-Tox	0.03	0.22	45.81	30	0.51	0.55	45.03	28
NEXUS	0.02	0.20	45.57	26	0.51	0.54	46.59	34
D-Tox	0.02	0.18	46.87	35	0.51	0.54	44.95	25
YODAsttest	0.02	0.20	45.95	31	0.51	0.55	46.09	33
UTSW_QBRC	0.02	0.22	46.56	34	0.51	0.55	46.07	32
D-Tox	0.02	0.19	47.50	39	0.51	0.54	45.76	31
TeamRoslin	0.03	0.26	45.59	27	0.51	0.54	48.30	43.5
MPIMG	0.02	0.22	46.42	33	0.50	0.55	48.13	41
Charlie's Minions	0.02	0.14	47.04	36	0.50	0.53	47.93	39
mlcb	0.02	0.18	47.58	40	0.51	0.54	47.52	35

amss2012	0.02	0.19	48.37	43	0.51	0.54	47.53	36
CytotoxicAvengers	0.02	0.16	47.23	37	0.50	0.54	48.30	43.5
PNNL	0.02	0.19	48.02	41	0.51	0.55	48.00	40
Battelle Team	0.02	0.21	48.97	48	0.51	0.55	47.64	37
FastRun	0.01	0.14	49.93	53	0.50	0.53	47.67	38
CompModel-IGIB	0.02	0.14	48.48	46	0.50	0.54	48.80	45
TeamRoslin	0.02	0.17	49.28	50	0.51	0.54	48.19	42
YODAsttest	0.02	0.19	47.36	38	0.50	0.55	50.96	54
CQB	0.02	0.16	48.46	45	0.50	0.55	49.26	48
CASSIS	0.02	0.20	49.29	51	0.51	0.55	49.01	46
ICOS Team	0.02	0.20	48.41	44	0.50	0.54	51.64	57
FastRun	0.01	0.18	49.99	54	0.50	0.54	49.04	47
UT_CCB	0.02	0.17	48.28	42	0.50	0.54	52.14	61
CASSIS	0.02	0.18	50.27	57	0.50	0.55	49.43	49
ICOS Team	0.02	0.20	49.12	49	0.50	0.54	51.87	58
mlcb	0.02	0.18	50.28	58	0.50	0.54	49.97	50
The fellowship of the ring	0.01	0.19	50.12	56	0.50	0.54	51.42	56
CompModel-IGIB	0.01	0.16	50.95	59	0.50	0.54	50.36	53
CQB	0.02	0.14	48.67	47	0.50	0.54	52.82	65
Purdue Xie	0.01	0.13	51.77	62	0.50	0.54	50.22	51
FIN&al	0.01	0.16	52.15	63	0.50	0.54	50.29	52
TeamRoslin	0.02	0.26	50.07	55	0.50	0.54	52.25	62
CytotoxicAvengers	0.01	0.16	49.84	52	0.50	0.53	53.68	67
ICOS Team	0.01	0.27	51.58	60	0.50	0.54	52.39	63
CompModel-IGIB	0.01	0.16	52.72	68	0.50	0.53	51.06	55
FastRun	0.01	0.16	52.44	64	0.50	0.53	52.09	59.5
UTSW_QBRC_km45	0.01	0.19	53.31	69	0.50	0.55	52.09	59.5
ICOS Team	0.01	0.19	51.61	61	0.50	0.54	54.99	71
CompModel-IGIB	0.01	0.16	52.62	67	0.50	0.54	52.94	66
CytotoxicAvengers	0.01	0.15	52.59	66	0.50	0.54	54.39	68
CompModel-IGIB	0.01	0.16	54.16	75	0.50	0.53	52.54	64
CytotoxicAvengers	0.01	0.15	53.36	70	0.50	0.54	55.02	72
The fellowship of the ring	0.01	0.18	53.47	72	0.50	0.54	54.70	70
sshh	0.01	0.15	53.52	73	0.50	0.53	54.42	69
mlcb	0.01	0.15	53.38	71	0.50	0.53	55.68	74
CytotoxicAvengers	0.00	0.15	53.58	74	0.50	0.54	55.18	73
PNNL	0.00	0.16	54.89	77	0.50	0.53	56.26	76
TeamDaniel	0.01	0.14	52.56	65	0.50	0.53	59.94	91
TeamDaniel	0.00	0.11	54.51	76	0.50	0.52	57.30	81
RNIgroup	0.00	0.14	55.88	81	0.50	0.54	56.46	78
mlcb	0.00	0.15	56.20	82	0.50	0.54	56.45	77
PNNL	0.00	0.14	55.31	78	0.50	0.54	57.48	82

PNNL	0.00	0.15	55.51	79	0.50	0.54	57.58	83
FastRun	0.00	0.16	56.44	84	0.50	0.53	57.20	80
PNNL	0.00	0.14	55.68	80	0.50	0.54	57.93	85
FastRun	-0.01	0.13	57.84	88	0.50	0.53	56.56	79
FIN&al	0.00	0.17	57.09	87	0.50	0.54	57.90	84
Charlie's Minions	0.00	0.15	56.86	85	0.50	0.53	58.91	87
bioinfoCIPF	NA	NA	98.94	99	0.50	0.53	55.72	75
FIN&al	0.00	0.17	56.41	83	0.50	0.53	60.48	92
mlcb	0.00	0.21	57.01	86	0.50	0.55	59.43	89
FIN&al	0.00	0.14	58.33	90	0.50	0.53	58.85	86
PCM	-0.01	0.12	59.75	91	0.50	0.52	59.15	88
UT_CCB	-0.01	0.12	58.22	89	0.50	0.53	60.63	93
FIN&al	-0.01	0.15	60.85	93	0.50	0.53	59.89	90
CQB	-0.01	0.15	60.70	92	0.50	0.54	61.41	94
BorRfLm	-0.01	0.15	62.04	94	0.50	0.54	63.49	96
Kaiju	-0.02	0.11	67.44	95	0.50	0.53	62.83	95
Kaiju	-0.03	0.12	68.61	96	0.50	0.53	66.26	97
Kaiju	-0.02	0.12	68.63	98	0.50	0.52	66.94	98
Kaiju	-0.02	0.12	68.62	97	0.50	0.53	68.20	99

<tables/SuppTable7/leaderboardSch1AllCompounds.pdf>