

# Tox21 Data Challenge 2014

# Final Subchallenge Leaderboard

Panel Winners **Y** 

Grand Challenge: Bioinf@JKU

Nuclear Receptor Panel: Bioinf@JKU-ensemble4

Stress Response Panel: Bioinf@JKU

Best Balanced Accuracy: AMAZIZ

#### | NR-AR (31/40 teams)

Team Name	Rank	AUC-ROC	Balanced Accuracy	Curve
<b>♀</b> dmlab	1	0.82752613	0.611933798	The state of the s
Bioinf@JKU-ensemble2	2	0.80799942	0.650116144	The state of the s
Bioinf@JKU	3	0.80712834	0.614547038	The state of the s
Bioinf@JKU-ensemble3	4	0.80466028	0.613675958	
Bioinf@JKU-ensemble4	5	0.80466028	0.609320557	To the state of th
VIF Innovations and CODDES	6	0.79696574	0.681910569	The state of the s
Bioinf@JKU-ensemble1	7	0.78694832	0.657084785	

Team Name	Rank	AUC-ROC	Balanced Accuracy	Curve
AMAZIZ	8	0.77003484	0.710801394	
RCC.ORG.RS	9	0.7630662	0.607578397	o o o o o o o o o o o o o o o o o o o
kibutz	10	0.75021777	<b>★</b> 0.735917538	To to the state of

# NR-AhR (35/40 teams)

Team Name	Rank	AUC-ROC	Balanced Accuracy	Curve
<b>₹</b> Bioinf@JKU	1	0.92788449	0.759406648	To Committee to Co
Bioinf@JKU-ensemble4	2	0.92431316	0.81612714	Control of the contro
Bioinf@JKU-ensemble3	3	0.92431316	0.766255963	Control of the contro
Bioinf@JKU-ensemble2	4	0.92399429	0.830756868	Solution of the control of the contr
Bioinf@JKU-ensemble1	5	0.92372644	0.78181679	Since the second
AMAZIZ	6	0.9133568	0.847771741	10 10 10 10 10 10 10 10 10 10 10 10 10 1
Т	7	0.9125405	★0.852758858	STATE OF THE PROPERTY OF THE P
microsomes	8	0.90078059	0.698362287	Control of the contro
StructuralBionformatics@Charite	9	0.89625265	0.814991964	10 and 10

Team Name	Rank	AUC-ROC	Balanced Accuracy	Curve
filipsPL	10	0.89259203	0.815782761	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1

# NR-AR-LBD (32/40 teams)

Team Name	Rank	AUC-ROC	Balanced Accuracy	Curve
₹ Bioinf@JKU-ensemble3	1	0.87913763	0.555531359	the state of the s
Bioinf@JKU-ensemble4	2	0.87913763	0.550304878	The state of the s
Bioinf@JKU	3	0.85017422	0.556402439	The state of the s
Bioinf@JKU-ensemble2	4	0.84984756	0.549433798	Topology
Т	5	0.84832317	0.604094077	10 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
AMAZIZ	6	0.8459277	0.593641115	10 10 10 10 10 10 10 10 10 10 10 10 10 1
dmlab	7	0.81859756	0.485191638	10 10 10 10 10 10 10 10 10 10 10 10 10 1
StructuralBionformatics@Charite	8	0.78887195	★0.650043554	O CONTROL OF CONTROL O
Bioinf@JKU-ensemble1	9	0.76361063	0.554660279	the state of the s
ToxFit	10	0.7565331	0.49912892	5 0 0 0 1 1 1 0

#### **IIII** NR-ER (33/40 teams)

Team Name	Rank	AUC-ROC	<b>Balanced Accuracy</b>	Curve
<b>♀</b> Bioinf@JKU-ensemble1	1	0.80976175	0.741049968	0) 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Bioinf@JKU-ensemble4	2	0.80877082	<b>★</b> 0.748956357	Tipoda
Bioinf@JKU-ensemble3	3	0.80877082	0.748703352	The state of the s
AMAZIZ	4	0.80626186	0.742061986	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
Bioinf@JKU-ensemble2	5	0.79854522	0.746805819	Silver Si
Bioinf@JKU	6	0.79270504	0.709487666	of the state of th
microsomes	7	0.78511491	0.620999367	The state of the s
Т	8	0.78359688	0.717077799	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
RCC.ORG.RS	9	0.7812355	0.686084756	Part of the control o
filipsPL	10	0.77113641	0.693991145	Olimbia di Control di

# | NR-ER-LBD (32/40 teams)

Team Name	Rank	AUC-ROC	Balanced Accuracy	Curve
<b>₹</b> microsomes	1	0.82732759	0.55	of the state of th

Team Name	Rank	AUC-ROC	Balanced Accuracy	Curve
Bioinf@JKU	2	0.81439655	0.634482759	Control of the contro
Bioinf@JKU-ensemble4	3	0.80737069	0.626724138	To do to
Bioinf@JKU-ensemble3	4	0.80737069	0.610344828	To to the state of
AMAZIZ	5	0.8062931	0.676724138	To
Т	6	0.80508621	0.701724138	To Care the Care
Bioinf@JKU-ensemble2	7	0.80107759	0.625862069	To do to
Bioinf@JKU-ensemble1	8	0.80043103	0.634482759	To to the state of
StructuralBionformatics@Charite	9	0.79788793	<b>★</b> 0.714655172	To
frozenarm	10	0.79047414	0.523275862	Control of the contro

# | NR-aromatase (32/40 teams)

Team Name	Rank	AUC-ROC	<b>Balanced Accuracy</b>	Curve
<b>♀</b> dmlab	1	0.83773793	0.562057574	13 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
Bioinf@JKU	2	0.83380525	0.631823187	Canada Ca
Т	3	0.82462902	0.726993865	To the state of th

Team Name	Rank	AUC-ROC	Balanced Accuracy	Curve
Bioinf@JKU-ensemble2	4	0.82119448	0.649284254	To the state of th
Bioinf@JKU-ensemble4	5	0.81914949	0.621598238	To the state of th
Bioinf@JKU-ensemble3	6	0.81914949	0.616957684	O Company
AMAZIZ	7	0.81873001	0.697734781	10 0 0 0 0 10 0 10 0 10 0 10 0 10 0 10
Bioinf@JKU-ensemble1	8	0.81791726	0.604137172	10 10 10 10 10 10 10 10 10 10 10 10 10 1
RCC.ORG.RS	9	0.79227623	0.729589429	O O O O O O O O O O O O O O O O O O O
StructuralBionformatics@Charite	10	0.78071417	★0.73666824	On the second of

# | MR-PPAR-gamma (31/40 teams)

Team Name	Rank	AUC-ROC	Balanced Accuracy	Curve
<b>₹</b> Bioinf@JKU-ensemble4	1	0.86085197	0.6447398	To the state of th
Bioinf@JKU-ensemble3	2	0.86085197	0.599837024	To Capada h
Bioinf@JKU-ensemble2	3	0.84913454	0.64299764	To the state of th
Bioinf@JKU-ensemble1	4	0.84017084	0.564965719	To the state of th
Bioinf@JKU	5	0.83929976	0.581094751	in the state of th

Rank	AUC-ROC	Balanced Accuracy	Curve
6	0.83137574	0.547516017	in the state of th
7	0.82994268	0.762953805	in the state of th
8	0.82168147	<b>★</b> 0.785180398	The state of the s
9	0.80299539	0.532258065	The state of the s
10	0.79127796	0.548387097	The state of the s
	6 7 8	6 0.83137574  7 0.82994268  8 0.82168147  9 0.80299539	6 0.83137574 0.547516017  7 0.82994268 0.762953805  8 0.82168147 ★0.785180398  9 0.80299539 0.532258065

# SR-ARE (33/40 teams)

Team Name	Rank	AUC-ROC	Balanced Accuracy	Curve
<b>₹</b> Bioinf@JKU	1	0.8399083	0.677209887	
Bioinf@JKU-ensemble4	2	0.83175069	0.715717079	Topological State of the Control of
Bioinf@JKU-ensemble3	3	0.83175069	0.650293255	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
Bioinf@JKU-ensemble2	4	0.83036587	<b>★</b> 0.728634269	To the state of th
Bioinf@JKU-ensemble1	5	0.82746823	0.650293255	Topological Control of the Control o
AMAZIZ	6	0.80472932	0.71522832	Truesday
microsomes	7	0.80448494	0.605257646	in the state of th

Team Name	Rank	AUC-ROC	Balanced Accuracy	Curve
Т	8	0.80134292	0.695887446	To the state of th
NCI	9	0.78347996	0.711073872	in the second se
dmlab	10	0.76794442	0.519340874	Topologia in the contract of t

# **SR-ATAD5** (30/40 teams)

Team Name	Rank	AUC-ROC	<b>Balanced Accuracy</b>	Curve
<b>₹</b> AMAZIZ	1	0.8281588	★0.741077866	Company of the compan
Т	2	0.813604	0.721611391	10 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
microsomes	3	0.81195926	0.53861752	The state of the s
dmlab	4	0.80037851	0.612427902	The state of the s
Bioinf@JKU	5	0.79262797	0.721431146	O CONTROL OF CONTROL O
Bioinf@JKU-ensemble2	6	0.78902307	0.707732516	Olympia in the state of the sta
Bioinf@JKU-ensemble4	7	0.78298486	0.706876352	O Tryoning in to
Bioinf@JKU-ensemble3	8	0.78298486	0.681957462	O CONTROL OF CONTROL O
Bioinf@JKU-ensemble1	9	0.77723955	0.667087239	

Team Name	Rank	AUC-ROC	Balanced Accuracy	Curve
StructuralBionformatics@Charite	10	0.75119412	0.690158616	The state of the s

# SR-HSE (30/40 teams)

Team Name	Rank	AUC-ROC	Balanced Accuracy	Curve
<b>₹</b> Bioinf@JKU-ensemble1	1	0.86471861	0.739795918	in the state of th
Bioinf@JKU-ensemble3	2	0.86290198	0.763373531	To the state of th
Bioinf@JKU-ensemble4	3	0.86290198	0.75487013	Tunnania is
Bioinf@JKU-ensemble2	4	0.86066017	0.75487013	Tuesday
NCI	5	0.8580705	0.771799629	To the state of th
Bioinf@JKU	6	0.85764533	0.596629561	The state of the s
dmlab	7	0.85548083	0.563079777	Topological to the state of the
StructuralBionformatics@Charite	8	0.8516543	<b>★</b> 0.798778602	in the state of th
AMAZIZ	9	0.84230056	0.747990105	Tuesday is a
Т	10	0.81060606	0.729514533	in the second se

#### **SR-MMP** (32/40 teams)

Team Name	Rank	AUC-ROC	Balanced Accuracy	Curve
T AMAZIZ	1	0.95022429	<b>★</b> 0.903571429	I i i i i i i i i i i i i i i i i i i i
dmlab	2	0.94584196	0.691770186	To the state of th
Bioinf@JKU-ensemble2	3	0.94156315	0.833540373	Fig. 1. Chapter 1. Cha
Bioinf@JKU	4	0.94052795	0.713664596	I de la companya de l
Bioinf@JKU-ensemble4	5	0.93826777	0.823136646	I de la companya de l
Bioinf@JKU-ensemble3	6	0.93826777	0.738664596	To the state of th
т	7	0.936853	0.869202899	To the state of th
Bioinf@JKU-ensemble1	8	0.93176329	0.74389234	in the state of th
filipsPL	9	0.9284334	0.836024845	10 10 10 10 10 10 10 10 10 10 10 10 10 1
RCC.ORG.RS	10	0.92016908	0.866252588	To the state of th

# SR-p53 (33/40 teams)

Team Name	Rank	AUC-ROC	Balanced Accuracy	Curve
<b>♀</b> dmlab	1	0.87991516	0.581018028	The state of the s

Team Name	Rank	AUC-ROC	<b>Balanced Accuracy</b>	Curve
Bioinf@JKU	2	0.8616755	0.662926829	On the state of th
Bioinf@JKU-ensemble1	3	0.8571368	0.662926829	Control of the contro
Bioinf@JKU-ensemble4	4	0.85641569	0.708250265	10 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Bioinf@JKU-ensemble3	5	0.85641569	0.651601273	10 10 10 10 10 10 10 10 10 10 10 10 10 1
Bioinf@JKU-ensemble2	6	0.85297985	0.747444327	the state of the s
Т	7	0.84680806	<b>★</b> 0.765005302	10 10 10 10 10 10 10 10 10 10 10 10 10 1
AMAZIZ	8	0.84349947	0.72407211	10 10 10 10 10 10 10 10 10 10 10 10 10 1
StructuralBionformatics@Charite	9	0.83406151	0.764135737	Table of the control
microsomes	10	0.82559915	0.522651113	

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