

Pacific Symposium on Biocomputing (PSB) 2022 Schedule

January 3-7, 2022, Big Island of Hawaii

Monday, January 3, 2022

Registration

8:30-9:30	Registration	Ballroom Prefunction
12:30-2:00	Registration	Ballroom Prefunction

Workshop #1 & #2

Plaza Ballroom

9:00-12:00 **Emerging Topics in Cancer Evolution**

Organizers: Mohammed El-Kebir, Quaid Morris, Layla Oesper, Cenk Sahinalp

1:30 - 4:30 **Image-based profiling: a powerful and challenging new data type**

Organizers: Gregory P. Way, Hannah Spitzer, Philip Burnham, Arjun Raj, Fabian Theis, Shantanu Singh, Anne E. Carpenter

Break

12:00-1:30 Lunch on own

Workshop #3 & #4

Salon 2&3

9:00- 12:00 **Genomic and Synthetic Biology Digital Biosecurity**

Organizers: Ravishankar K. Iyer, Zbigniew T. Kalbarczyk, Nina Alli, Corey M. Hudson, Nicholas D. Pattengale

1:30-4:30 **Social, Technical, and Ethical Challenges in Biomedical Data Privacy**

Organizers: Gamze Gursoy, Steven Brenner, Bradley Malin, Barbara Koenig

Reception

Croquet Lawn

5:00-6:00 Opening Reception
Sponsored by the Cleveland Institute for Computational Biology

Dinner

6:00- Dinner on own

Please wear your PSB name tag and lanyard for admission to all events and hosted meals.

January 5, 2022

Pacific Symposium on Biocomputing (PSB) 2022 Schedule

January 3-7, 2022, Big Island of Hawaii

Tuesday, January 4, 2022

Registration

7:30-9:00	Registration	Ballroom Prefunction
10:30-11:30	Registration	Ballroom Prefunction
12:00-1:30	Registration	Ballroom Prefunction

Breakfast

7:30-8:45	PSB Breakfast	Ballroom Courtyard
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Welcome

8:45-9:00	Welcome – Teri Klein	Salon 2&3
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Session 1

Salon 2&3

Precision Medicine: Using Artificial Intelligence to Improve Diagnostics and Healthcare

Co-chairs: Steven E. Brenner, Martha L. Bulyk, Jonathan Chen, Dana C. Crawford, Roxana Daneshjou, Samuel G. Finlayson, Łukasz Kidziński

9:00-9:15	Introduction
9:15-9:30	<i>Interpretable Deep Learning Prediction of 3D Assessment of Cardiac Function</i> <u>Grant Duffy</u> , Ishan Jain, Bryan He, David Ouyang
9:30-9:45	<i>Hierarchical Gaussian Processes and Mixtures of Experts to Model COVID-19 Patient Trajectories</i> <u>Sunny Cui</u> , Elizabeth C. Yoo, Didong Li, Krzysztof Laudanski, Barbara E. Engelhardt
9:45-10:00	<i>De novo Prediction of Cell-Drug Sensitivities Using Deep Learning-based Graph Regularized Matrix Factorization</i> <u>Shuangxia Ren</u> , Yifeng Tao, Ke Yu, Yifan Xue, Russell Schwartz, Xinghua Lu
10:00-10:15	<i>Clinical Recommender Algorithms to Simulate Digital Specialty Consultations</i> Morteza Noshad, Ivana Jankovic, <u>Jonathan H. Chen</u>
10:15-10:30	<i>A Method for Localizing Non-Reference Sequences to the Human Genome</i> <u>Brianna Sierra Chrisman</u> , Kelley M Paskov, Chloe He, Jae-Yoon Jung, Nate Stockham, Peter Yigitcan Washington, Dennis Paul Wall

Break

10:30-10:50	Break
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Keynote

Salon 2&3

10:50-12:00	<i>Decoding the Genome to Uncover Molecular Basis of Human Disease</i> Olga Troyanska with introduction by Russ Altman
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Lunch

Ballroom Courtyard

12:00-2:00	PSB Hosted Lunch
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Tuesday, January 4, 2022 (*continued*)

Workshop #5

Salon 2&3

2:00-5:00

Packaging Biocomputing Software to Maximize Distribution and Reuse

Co-chairs: William S. Bush, Christian Darabos, Brett Beaulieu-Jones, Nicholas Wheeler

Dinner

5:00-

Dinner & Evening on own

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Pacific Symposium on Biocomputing (PSB) 2022 Schedule

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Wednesday, January 5, 2022

Registration		Ballroom Prefunction
7:15-8:30	Registration	
Breakfast		Ballroom Courtyard
7:15-8:30	PSB Breakfast	
Announcements		Salon 2&3
8:30-8:40	Morning Announcements – Marylyn Ritchie	
TERI Talks		Salon 2&3
8:40-9:10	Russ Altman, Stanford University	
9:10-9:40	Lawrence Oloff, Palo Alto Medical Foundation	
Session 1 (continued)		Salon 2&3
	Precision Medicine: Using Artificial Intelligence to Improve Diagnostics and Healthcare	
	Co-chairs: Steven E. Brenner, Martha L. Bulyk, Jonathan Chen, Dana C. Crawford, Roxana Daneshjou, Samuel G. Finlayson, Łukasz Kidziński	
9:40-9:55	<i>netCRS: Network-based comorbidity risk score for prediction of myocardial infarction using biobank-scaled PheWAS data</i> <u>Yonghyun Nam</u> , Sang-Hyuk Jung, Anurag Verma, Vivek Sriram, Hong-Hee Won, Jae-Seung Yun, Regeneron Genetics Center, Dokyoon Kim	
9:55-10:10	<i>CloudPred: Predicting Patient Phenotypes from Single-cell RNA-seq</i> <u>Bryan He</u> , Matthew Thomson, Meena Subramaniam, Richard Perez, Chun Jimmie Ye, James Zou	
10:10-10:25	<i>Nonlinear post-selection inference for genome-wide association studies</i> <u>Lotfi Slim</u> , Clément Chatelain, Chloé-Agathe Azencott	
10:25-10:40	<i>Evaluation of Sex-Aware PrediXcan Models for Predicting Gene Expression</i> Emily Mahoney, Vaibhav Janve, Timothy J. Hohman, <u>Logan Dumitrescu</u>	
10:40-10:55	<i>An Investigation of the Knowledge Overlap between Pharmacogenomics and Disease Genetics</i> <u>Binglan Li</u> , Michelle Whirl-Carrillo, Matt W. Wright, Larry Babb, Heidi L. Rehm, Teri E. Klein	
Break		
10:55-11:10	Break	
Discussion Session		Salon 2&3
11:10-12:10	Precision Medicine: Using Artificial Intelligence to Improve Diagnostics and Healthcare	

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Pacific Symposium on Biocomputing (PSB) 2022 Schedule

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Wednesday, January 5, 2022 (continued)

Poster Session Lunch Salon 1 and Ballroom Courtyard

12:10-2:10 Poster Session with Lunch
(Posters on ODD numbered boards presented from 12:10-1:10)
(Posters on EVEN numbered boards presented from 1:10-2:10)

Session 2 Salon 2&3

AI-driven Advances in Modeling of Protein Structure

Co-chairs: Krzysztof Fidelis, Sergei Grudinin

2:10-2:20 Introduction

2:20-2:40 Invited Talk: Sergei Grudinin

2:40-2:55 *Training data composition affects performance of protein structure analysis algorithms*

Alexander Derry, Kristy A. Carpenter, Russ B. Altman

2:55-3:10 *Transferability of Geometric Patterns from Protein Self-Interactions to Protein-Ligand Interactions*

Antoine Koehl, Milind Jagota, Dan D. Erdmann-Pham, Alexander Fung, Yun S. Song

3:10-3:25 *Interpreting Potts and Transformer Protein Models Through the Lens of Simplified Attention*

Nicholas Bhattacharya, Neil Thomas, Roshan Rao, Justas Dauparas, Peter K. Koo, David Baker, Yun S. Song, Sergey Ovchinnikov

3:25-3:40 *Side Chain Packing Using SE(3)-Transformer*

Akhil Jindal, Yimin Zhu, Sergey Kotelnikov, Rezaul Chowdhury, Sandor Vajda, Dzmitry Padhorny, Dima Kozakov

3:40-3:55 *DeepVASP-E: A Flexible Analysis of Electrostatic Isopotentials for Finding and Explaining Mechanisms that Control Binding Specificity*

Felix M. Quintana, Zhaoming Kong, Lifang He, Brian Y. Chen

Discussion Session Salon 2&3

3:55-4:55 **AI-driven Advances in Modeling of Protein Structure**

Dinner

4:55- Dinner & Evening on own

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Pacific Symposium on Biocomputing (PSB) 2022 Schedule

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Thursday, January 6, 2022

Breakfast		Ballroom Courtyard
7:15-8:30	PSB Breakfast	
Announcements		Salon 2&3
8:30-8:40	Morning Announcements – Larry Hunter	
TERI Talks		Salon 2&3
8:40-9:10	Philip Bourne, University of Virginia	
9:10-9:40	Alex Wagner, Nationwide Children's	
Session 3		Salon 2&3
	Human Intrigue: Meta Analysis Approaches for Big Questions with Big Data	
	Co-chairs: Carly A. Bobak, Meghan E. Muse, Kristine A. Giffin, Derek A. Williamson, Dennis P. Wall, Casey S. Greene, Jason Moore	
9:40-9:50	Introduction	
9:50-10:05	<i>Multitask group Lasso for Genome Wide association Studies in diverse populations</i> <u>Asma Nouria</u> , Chloé-Agathe Azencott	
10:05-10:20	<i>Improving QSAR Modeling for Predictive Toxicology using Publicly Aggregated Semantic Graph Data and Graph Neural Networks</i> <u>Joseph D. Romano</u> , Yun Hao, Jason H. Moore	
10:20-10:35	<i>CAMML: Multi-Label Immune Cell-Typing and Stemness Analysis for Single-Cell RNA-sequencing</i> <u>Courtney Schiebout</u> , H. Robert Frost	
10:35-10:50	<i>Reconciling Signaling Pathway Databases with Network Topologies</i> Tobias Rubel, <u>Pramesh Singh</u> , Anna Ritz	
10:50-11:10	Invited Talk: Purvesh Khatri	
Discussion Session		Salon 2&3
11:10-12:10	Human Intrigue: Meta Analysis Approaches for Big Questions with Big Data	
Awards		Salon 2&3
12:10-12:30	Parasite & Symbiont Awards	
Lunch		
12:30-5:30	Lunch and Afternoon on Own (Networking Time)	
Dinner		Coconut Grove
5:30-7:15	PSB Dinner Banquet	
Keynote		Salon 2&3
7:30-8:30	Carbon versus Silicon: Professional Ethics Rob Reich with introduction by Russ Altman	

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Pacific Symposium on Biocomputing (PSB) 2022 Schedule

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Friday, January 7, 2022

Breakfast		Ballroom Courtyard
7:30-8:30	Breakfast	
Closing		Salon 2&3
8:30-8:40	Closing Announcements – Larry Hunter	
Session 4		Salon 2&3
	Big Data Imaging Genomics: Reproducible Findings, Individual Predictions, and Clinical Decisions	
	Co-chairs: Peter Kochunov, Li Shen, John Darrell Van Horn, Paul M Thompson	
8:40-8:50	Introduction	
8:50-9:10	Invited Talk: Hongtu Zhu	
9:10-9:25	<i>A new Mendelian Randomization method to estimate causal effects of multivariable brain imaging exposures</i> Chen Mo, Zhenyao Ye, Hongjie Ke, Tong Lu, Travis Canida, Song Liu, Qiong Wu, Zhiwei Zhao, Yizhou Ma, L. Elliot Hong, Peter Kochunov, Tianzhou Ma, <u>Shuo Chen</u>	
9:25-9:40	<i>Identifying highly heritable brain amyloid phenotypes through mining Alzheimer's imaging and sequencing biobank data</i> <u>Jingxuan Bao</u> , Zixuan Wen, Mansu Kim, Xiwen Zhao, Brian N. Lee, Sang-Hyuk Jung, Christos Davatzikos, Andrew J. Saykin, Paul M. Thompson, Dokyoon Kim, Yize Zhao, Li Shen, for the Alzheimer's Disease Neuroimaging Initiative	
9:40-9:55	<i>Separating Clinical and Subclinical Depression by Big Data Informed Structural Vulnerability Index and Its impact on Cognition: ENIGMA Dot Product</i> <u>Peter Kochunov</u> , Yizhou Ma, Kathryn S. Hatch, Lianne Schmaal, Neda Jahanshad, Paul M. Thompson, Bhim M. Adhikari, Heather Bruce, Joshua Chiappelli, Andrew Van der vaart, Eric L. Goldwaser, Aris Sotiras, Tianzhou Ma, Shuo Chen, Thomas E. Nichols, L. Elliot Hong	
Discussion Session		Salon 2&3
9:55-10:55	Big Data Imaging Genomics: Reproducible Findings, Individual Predictions, and Clinical Decisions	

PSB over--see you next year!

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January 5, 2022