KEYSTONE SYMPOSIA
on Molecular and Cellular Biology

Antibodies as Drugs (J7)

Scientific Organizers: Pierre Bruhns, Esther Breij and David P. Humphreys

Sponsored by Genentech, Inc., Genmab A/S and Regeneron Pharmaceuticals, Inc.

Computational Design and Modeling of Biomolecules (J8)

Scientific Organizers: Timothy Whitehead, Nir London, Roberto A. Chica and Birte Höcker

January 30-February 2, 2022 • Keystone Resort • Keystone, CO, USA

Sponsored by Genmab A/S

Global Health Travel Award Deadline: January 10, 2022 / Scholarship Deadline: October 14, 2021 / Abstract Deadline: October 21, 2021 / Discounted Registration Deadline: November 30, 2021

SUNDAY, JANUARY 30

Arrival and Registration

MONDAY, JANUARY 31

Welcome and Keynote Address (J7)

Erica Ollmann Saphire, La Jolla Institute for Immunology, USA
Differential Features of SARS-CoV-2 Therapeutic Antibodies

Welcome and Keynote Address (J8)

David Baker, University of Washington, USA
De novo Design of Function

Therapeutic Antibodies from Patients (J7)

Adrian C. Hayday, King's College London School of Medicine, UK
Anti-Cytokine Abs from Autoimmune Patients

Stephen Quake, Stanford University, USA
Isolation of Rare Human Plasma Cells: Showcasing Anti-Peanut IgE Antibodies

Natalia Freund, Tel Aviv University, Israel
Human-Isolated Antibodies Targeting Mycobacterium Tuberculosis

Kelsey Pilewski, Vanderbilt University, USA
Short Talk: Functional HIV-1/HCV Cross-reactive Antibodies Isolated from a Chronically Co-infected Donor

Matteo Broketa†, Institut Pasteur, France
Short Talk: High throughput Affinity Repertoire Mapping of Plasmablasts against SARS-COV2 RBD and Variants following mRNA Vaccination of Naïve and COVID-19-Convalescent Individuals

Jarrod J. Mousa, University of Georgia, USA
Short Talk: Broadly Reactive Anti-Pneumococcal Antibodies for Disease Treatment

Computational de novo Design of Biomolecules (J8)

Jane S. Richardson, Duke University, USA
A Brief History of Protein Design

Stephen L. Mayo, Caltech, USA
Computational Design of Novel Antibody Small Molecule Conjugates

Tanja Kortemme, University of California, San Francisco, USA
Computational Design of New Molecular Geometries and Ligand-Controlled Functions

Anastassia A. Vorobieva, VIB-VUB, Belgium
Short Talk: De Novo Design of Pore-Forming Transmembrane beta-barrels

Alexandra K. Van Hall-Beauvais, École polytechnique fédérale de Lausanne, Switzerland
Short Talk: De Novo Design of Site-specific Protein Binders Using Learned Surface Fingerprints

Anum Glasgow, Columbia University, USA
Short Talk: Biophysical Requirements for Affinity and Stability in Engineered Anti-SARS-CoV-2 Receptor Traps

Workshop (J7)

Xiaoying Yu, The Scripps Research Institute, USA
Asymmetric and Non-Stoichiometric Recognition Results in Broad Protection Against Ebolaviruses by a Two-Antibody Cocktail

Franziska Heckel, University of Southampton, UK
CD27 Antibody Mediated Agonism is Facilitated through Epitope-Dependent Receptor Clustering and can be Augmented through Fc-Engineering

Linya Wang, Twist Bioscience, USA
Functional ADORA2A Antibodies Demonstrate Antagonistic and Tumor Suppression Activities

Fergus R. Byrne, Boehringer Ingelheim, USA
An Anti Human LAIR-1 Agonistic Monoclonal Antibody Requires Fc Receptor Engagement for Functional Efficacy

Jiachen Huang, University of Georgia, USA
Therapeutic Monoclonal Antibodies for Human Metapneumovirus

Daniel Leventhal, Generate Biomedicines, USA
Computational Directed Improvements in Developability and Immunogenicity for Therapeutic Antibodies

Taylor Engdahl, Vanderbilt University Medical Center, USA
Broadly Neutralizing Hantavirus Antibodies Target an Antigenic Site Spanning the Gn/Gc Heterodimer

Antibodies from Within: Vaccination and Delivery Technologies (J7)

Matthieu Mahévas, Institut Necker Enfants Malades, INSERM, France
Maturation of Memory B cells after SARS-CoV2 Infection and mRNA Vaccine

Peter D. Kwong, NIAID, National Institutes of Health, USA
Anti-HIV and Anti-Malarial Antibodies Elicited by Vaccination

Andrea Carfi, Moderna, USA
Antibody-Inducing mRNA-Based Vaccine for COVID-19: 1 Year Experience in Humans

Ronald C. Desrosiers, University of Miami Miller School of Medicine, USA
AAV Delivery of Antibodies for Long-Term Protection

Tineke Cantaert, Institut Pasteur Cambodia, Cambodia
Human Anti-Dengue Antibody Responses

Blake M. Hauser, Harvard Medical School, USA
Short Talk: Rationally Designed Immunogens Enable Immune Focusing Following SARS-CoV-2 Spike Imprinting

Elaine C. Chen, Vanderbilt University, USA
Short Talk: Systematic Analysis of the Private and Public Ebola Specific Antibody Response

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Repurposing Proteins for Binding and Catalysis (J8)

William F. DeGrado, University of California, San Francisco, USA
de novo Design of Binding Proteins and Catalysts

Birte Höcker, University of Bayreuth, Germany
Evolution and Design of Proteins

Dek Woolfson, University of Bristol, UK
Exploring the Dark Space of Protein Structure and Function through Rational and Computational Design

Neil P. King, University of Washington, USA
Computational Design of Self-Assembling Protein Nanomaterials for Medical Applications

Pranam Chatterjee, MIT Media Lab, USA
Short Talk: De Novo Design of Potent Anti-CRISPR Proteins

Rodney Park, University of North Carolina at Chapel Hill, USA
Short Talk: Improving Enzymatic Efficiency by more than 1000-Fold through Computational Interface Design of a Substrate Recruitment Domain

Poster Session 1

TUESDAY, FEBRUARY 1

New Targets and Tools (J7)

David P. Humphreys, UCB Pharma, UK
IgG FcRn Blockade Therapeutics

Esther Breij, Genmab, Netherlands
Enhanced IgG Hexamerization for Increased Therapeutic Antibody Potency

Amita Datta-Mannan, Eli Lilly & Company, USA
FcRn Binding Ab Mutants, Peptide Fusions and Glycan Effects

Pierre Bruhns, Institut Pasteur, France
Human Autoimmune Plasma Cell Repertoires

Stefan Gerhardy, Genentech, USA
Short Talk: Allosteric Inhibition of HtrA1 Activity by a Conformational "Lock" Mechanism to Treat Age-related Macular Degeneration

Andrea Shiakolas, Vanderbilt University, USA
Short Talk: Rapid and Efficient Discovery of Potently Neutralizing SARS-CoV-2 Antibodies Using LIBRA-seq with Ligand Blocking

Energy Landscape Search for Affinity and Specificity (J8)

Amy E. Keating, Massachusetts Institute of Technology, USA
Mapping Peptide Binding Specificity Space

Roberto A. Chica, University of Ottawa, Canada
Computational Design of Protein Energy Landscapes

Bruce Donald, Duke University, USA
Algorithms for Ensemble-Based Computational Protein Design

Sophie Barbe, Université de Toulouse, France
Search Algorithms in Protein Design

Jilliane Bruffey, University of Washington, USA
Short Talk: Design of Conditionally Active Proteins for the Treatment of Solid Tumors

Nick Wells†, Wesleyan University, USA
Short Talk: Computational Design of Allosterically Acting Mutations using MD Simulations and Rosetta

Clara Tabea Schoeder, Leipzig University Medical Faculty, Germany
Short Talk: Structure-Based Immunogen Design to Target Ebola and Marburg Virus Glycoprotein Epitopes

Prediction and Design of Protein Ligand Interactions (J8)

Brian K. Shoichet, University of California, San Francisco, USA
Ultra-Large Library Docking for Discovering New Chemotypes

Nir London, Weizmann Institute of Science, Israel
Designing Covalent Inhibitors

Xavier Barril, Gain Therapeutics, Spain
High-Throughput Virtual Dissociation Experiments: Application to Fragment Screening

Ora Furman, Hebrew University, Hadassah Medical School, Israel
Peptides as Far as the Eye Can See

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Peptides as Far as the Eye Can See

Simon Kretschmer, University of California San Francisco, USA
Short Talk: Design of Multi-layer Protein Switches Controlled by FDA-Approved Small-Molecule Drugs

Patrick Kelly, Arizona State University, USA
Short Talk: Computational Design of a Protein-Based Fluorescent Metal Sensor

The Rise of Bispecifics (J7)

Stefan Weigand, F. Hoffmann La Roche AG, Switzerland
Complex Biologics from Roche's Pipeline

Matthew Sleeman, Regeneron Pharmaceuticals, Inc., USA
Costimulatory Bispecifics Antibodies

Mark S. Dennis, Denali Therapeutics, USA
BBB Crossing Bispecific Abs

Bruce Keyt, IGM Biosciences, USA
IgM Bispecifics and Multimers as Therapeutics

Natasa Vukovic, University of Edinburgh, UK
Short Talk: Development of Bispecific IgE Antibodies

Rony Dahan, Weizmann Institute of Science, Israel
Short Talk: Cell Type-selective Bispecific Antibodies to Separate Toxicity and Efficacy of Agonistic Antibodies

Poster Session 2

WEDNESDAY, FEBRUARY 2

Keynote Address (Joint)

Charlotte Deane, University of Oxford, UK
Deep Learning based on Ab Sequences and Structure Information

Repertoires, Learning and in Silico Design (Joint)

Arvind Sivasubramanian, Adimab LLC, USA
Computational Modeling and Design of Antibody Function

Sai T. Reddy, ETH Zurich, Switzerland
Engineering an Antigen-Binding Protein by Deep Learning-Guided Directed Evolution

Byung-Ha Oh, Korea Advanced Institute of Science & Technology, South Korea
Short Talk: Computational Design of a Neutralizing Antibody with Pico- to Femto-Molar Binding Affinity for all SARS-CoV-2 Variants of Concern

Reda Rawi, National Institute of Allergy and Infectious Diseases, NIH, USA
Short Talk: In silico Improvement of Highly Protective Anti-malarial Antibodies

Novel Therapeutic Antibodies in the Clinic (J7)

Cecile Geuijen, Merus NV, Netherlands
Targeting T/NK Costimulatory Receptors in Oncology (4-1BBxPD-L1 Bispecific Antibody)

Eric Vivier, Aix Marseille University and Inna Pharma, France
Exploiting NK Cells to Induce Anti-Tumor Response in Preclinical and Clinical Setting

Neil Brewis, F-star Biotechnology Ltd., UK
Immuno-Oncology Therapeutics (including OX40x4-1BB Bispecifics)

Christos Kyratsous, Regeneron Pharmaceuticals Inc, USA
Anti-Covid-19 Therapeutic mAbs: Design and Results One Year After

Tibor Keler, Celldex Therapeutics, Inc., USA
Short Talk: Development of the Antagonist KIT Antibody CDX-0159 for Mast Cell Driven Diseases

Machine Learning for Design of Enhanced Therapeutics and Biocatalysts (J8)

Timothy Whitehead, University of Colorado Boulder, USA
One-Shot Design and Engineering of Portable in vitro and in vivo Biosensors

Joanna Slusky, University of Kansas, USA
Machine Learning for Accelerating the Design of Metalloenzymes.

Daniela Grabs, Arzeda Corp, USA
Designer Enzymes to Deliver Performance Chemicals and Materials

Bruno Emanuel Correia, École Polytechnique Fédérale de Lausanne, Switzerland
Deciphering Interaction Fingerprints from Protein Molecular Surfaces using Geometric Deep Learning

Possu Huang†, University of California, San Francisco, USA
Short Talk: Epitope-Specific Antibody Design via Deep Learning-Based Structural Modeling

Meeting Wrap-Up: Outcomes and Future Directions (Organizers) (J7)

Meeting Wrap-Up: Outcomes and Future Directions (Organizers) (J8)

THURSDAY, FEBRUARY 3

Departure