| B Break D Discu | ussion [| I Invited Talk L Lightning talks S Social space T Talk | |
|-----------------------------|----------|--|---------------|
| OCTOBER 5 · MONDA | ΛY | | |
| PINNED 01:00 – 01:45 | I | CellDesigner: A modeling tool for biochemical networks Speakers: Akira Funahashi | Room 1 |
| 01:45 – 02:00 | Т | A modular, thermodynamic approach for constructing large-scale kinetic models in systems biology Speakers: Michael Pan | Room 1 |
| 02:00 – 02:15 | Т | Open Source and Sustainability Speakers: Jacob Barhak | Room 1 |
| 02:15 - 02:30 | Т | Physiome - Make your model publications discoverable, reproducible, and reusable. Speakers: Karin Lundengård | Room 1 |
| 02:30 - 02:45 | D | Discussion | Room 1 |
| 02:45 - 03:00 | В | Break | Room 1 |
| 03:00 – 03:15 | Т | OpenCOR: how to enable reproducible science using community standards and tools Speakers: Alan Garny | Room 1 |
| 03:15 - 03:30 | Т | CelIML 2.0 Speakers: David Nickerson | Room 1 |
| 03:30 - 03:45 | Т | Implementing OMEX metadata v1.1 Speakers: John Gennari | Room 1 |
| 03:45 - 04:00 | D | Discussion | Room 1 |
| PINNED 04:00 – 06:00 | S | Social space/BREAK | Room 1 |
| PINNED 06:00 – 06:45 | I | COVID-19 Disease Map: the key role of standards in community-driven development of systems biole disease models Speakers: Marek Ostaszewski | ogy Room 1 |
| 06:45 - 07:00 | Т | PEtab – Interoperable Specification of Parameter Estimation Problems in Systems Biology Speakers: Daniel Weindl | Room 1 |
| 07:00 – 07:15 | Т | Spatial Model Editor Speakers: Liam Keegan | Room 1 |
| 07:15 – 07:30 | Т | pyABC: likelihood-free inference Speakers: Emad Alamoodi | Room 1 |
| 07:30 – 07:45 | D | Discussion | Room 1 |
| 07:45 - 08:00 | В | Break | Room 1 |
| 08:00 – 08:15 | Т | FAIRDOM: standard compliant data and model management Speakers: Olga Krebs | Room 1 |
| 08:15 – 08:30 | Т | FAIR principles in literature-based kinetic modelling Speakers: Christoff Odendaal | Room 1 |
| 08:30 - 08:45 | T | Stochastic Modelling and Prediction of the COVID-19 Speakers: Joab Odhiambo | Room 1 |
| 08:45 - 09:00 | D | Discussion | Room 1 |
| PINNED 09:00 - 10:00 | S | Social space/BREAK | Room 1 |

| 10.15 - 10.20 | 10:00 – 10:15 | T Automated inference of Boolean models from molecular interaction maps using CaSQ Speakers: Anna Niarakis | Room 1 |
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| Data Speakers Witer Vieira Speakers Steven Verrouysse Speakers Steven Verrouysse Speakers Steven Verrouysse Speakers Witerouysse Speakers Wi | 10:15 – 10:30 | | Room 1 |
| 11:00 - 11:15 | 10:30 – 10:45 | Data | _ |
| 11:15 - 11:30 | 10:45 – 11:00 | D Discussion | Room 1 |
| 11.30 - 11.45 | 11:00 – 11:15 | B Break | Room 1 |
| 11.45 - 12.00 | 11:15 – 11:30 | | Room 1 |
| 12:00 - 12:15 D D D D D D D D D | 11:30 – 11:45 | | Room 1 |
| Information and data standards used at Ginkgo Bioworks Speakers: Ariel Hecht | 11:45 – 12:00 | | Room 1 |
| PINNED 12:15 - 13:00 Speakers: Ariel Hecht 12:15 - 13:00 Social space/BREAK Room 1 13:00 - 14:00 Room 1 14:10 Room 1 14:15 Room 1 14:15 - 14:30 Room 1 14:30 - 14:45 Room 1 15:00 - 15:15 Room 1 15:00 - 15:45 Room 1 15:00 - 15:15 | 12:00 – 12:15 | D Discussion | Room 1 |
| Name | | · · · · · · · · · · · · · · · · · · · | Room 1 |
| Speakers: Isabel Marleen Pötzsch 14:15 – 14:30 T SABIO-RK: Curation and Visualization of Reaction Kinetics Data Speakers: Ulrike Wittig 14:30 – 14:45 T EnzymeML – an SBML-based data exchange format for biocatalysis and enzymology Room 1 15:45 – 15:00 D Discussion Room 1 15:15 – 15:30 T Stochastic Differential Equations and their Application in Systems Biology Room 1 15:30 – 15:45 T Towards in silico approaches for personalized medicine – Recommendations for verifying and validating predictive computational models in EU collaborative research Room 1 15:45 – 16:00 T Automated Extraction of Implicit Molecular Structure from Reaction Network Models Room 1 16:00 – 16:15 D Discussion Room 1 1 TBA Speakers: Nathan Hillson 1 TBA Speakers: Nathan Hillson 1 TBA Speakers: Nathan Hillson Room 1 | | S Social space/BREAK | Room 1 |
| Speakers: Ulrike Wittig 14:30 – 14:45 T EnzymeML – an SBML-based data exchange format for biocatalysis and enzymology Room 1 Speakers: Juergen Pleiss 14:45 – 15:00 D Discussion Room 1 15:00 – 15:15 B Break Room 1 15:15 – 15:30 T Stochastic Differential Equations and their Application in Systems Biology Room 1 Speakers: Stefan Hoops Room 1 Speakers: Stefan Hoops Room 1 Speakers: Catherine Collin T Towards in silico approaches for personalized medicine – Recommendations for verifying and validating predictive computational models in EU collaborative research Room 1 Speakers: Catherine Collin Room 1 Speakers: Ali Sinan Saglam Room 1 Taka Room 1 Taka Room 1 Speakers: Nathan Hillson Speakers: Nathan Hillson Room 1 Taka | 14:00 – 14:15 | | Room 1 |
| 14:45 - 15:00 D Discussion Room 1 | 14:15 – 14:30 | | Room 1 |
| 15:00 - 15:15 B Break Room 1 | 14:30 – 14:45 | | Room 1 |
| 15:15 – 15:30 T Stochastic Differential Equations and their Application in Systems Biology Speakers: Stefan Hoops 15:30 – 15:45 T Towards in silico approaches for personalized medicine – Recommendations for verifying and validating predictive computational models in EU collaborative research Speakers: Catherine Collin 15:45 – 16:00 T Automated Extraction of Implicit Molecular Structure from Reaction Network Models Speakers: Ali Sinan Saglam 16:00 – 16:15 D Discussion Room 1 PINNED 16:15 – 17:00 S Social space/BREAK Room 1 PINNED 17:00 – 18:00 Opening session Room 1 | 14:45 – 15:00 | D Discussion | Room 1 |
| Speakers: Stefan Hoops 15:30 - 15:45 T Towards in silico approaches for personalized medicine - Recommendations for verifying and validating predictive computational models in EU collaborative research Room 1 | 15:00 – 15:15 | B Break | Room 1 |
| predictive computational models in EU collaborative research Speakers: Catherine Collin 15:45 – 16:00 T Automated Extraction of Implicit Molecular Structure from Reaction Network Models Speakers: Ali Sinan Saglam 16:00 – 16:15 D Discussion Room 1 PINNED 1: TBA Speakers: Nathan Hillson S Social space/BREAK Room 1 PINNED 17:00 – 18:00 Opening session Room 1 | 15:15 – 15:30 | | Room 1 |
| Speakers: Ali Sinan Saglam 16:00 – 16:15 D Discussion Room 1 | 15:30 – 15:45 | predictive computational models in EU collaborative research | _ |
| PINNED 16:15 – 17:00 S Social space/BREAK PINNED 17:00 – 18:00 Opening session Room 1 PINNED | 15:45 – 16:00 | · | Room 1 |
| PINNED Speakers: Nathan Hillson S Social space/BREAK PINNED 17:00 – 18:00 Opening session PINNED | 16:00 – 16:15 | D Discussion | Room 1 |
| PINNED 17:00 – 18:00 Opening session Room 1 PINNED | | | Room 1 |
| PINNED | | S Social space/BREAK | Room 1 |
| | | Opening session | Room 1 |

| PINNED 18:15 – 19:00 | Novel technologies for systematically building and simulating whole-cell models Speakers: Jonathan Karr | Room |
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| 19:00 – 19:30 | L Lightning talks (1) Speakers: Paul Stapor, Mudasir Shaikh, Michael Blinov, Gonzalo Vidal, Adrien Rougny, Joseph Hellerstein | Room |
| 19:30 – 19:45 | D Discussion | Room |
| 19:45 – 20:00 | B Break | Room |
| 20:00 – 20:30 | L Lightning talks (2) Speakers: Malik-Sheriff, Rahuman S., Eirini Tsirvouli, Hugh Sorby, Adel Heydarabadipour, Joab Odhiambo | Room |
| 20:30 – 21:00 | D Wrap-ups // Discussion | Room |
| PINNED 21:00 – 21:45 | Putting energy into systems biology: biophysical models of cell systems for understanding, simulation design Speakers: Edmund Crampin | on and Room |
| 21:45 – 22:00 | T A thermodynamic Model of EGFR and ERK Signaling explains Adaptive and Genetic Resistance in Melanoma Speakers: Fabian Fröhlich | Room [·] |
| 22:00 – 22:15 | T The Systems Biology Graphical Notation: a standardised representation of biological maps Speakers: Michael Blinov | Room |
| 22:15 – 22:30 | T BioSimulators: a registry of containerized biosimulation tools with standard interfaces that enhance to reuse of biomodels Speakers: Bilal Shaikh | t he Room 1 |
| 22:30 – 22:45 | D Discussion | Room 1 |
| 22:45 – 23:00 | B Break | Room |
| 23:00 – 23:15 | T Datanator: an integrated database of molecular data for quantitatively modeling cellular behavior Speakers: Lian Zhouyang | Room |
| 23:15 – 23:30 | T SBViper: Verification Testing of Kinetics Models in Systems Biology Speakers: Joseph L Hellerstein | Room |
| 23:30 – 23:45 | T pyPESTO: A python package for Parameter Estimation and Uncertainty Quantification Speakers: Jakob Vanhoefer | Room |
| 23:45 – 00:00 | D Discussion | Room |
| | | |

I Invited Talk **B** Break **D** Discussion S Social space T Talk **OCTOBER 6 • TUESDAY** S Social space/BREAK Room 1 **PINNED** 00:00 - 01:0001:00 - 01:15T (Replay) Automated inference of Boolean models from molecular interaction maps using CaSQ Room 1 Speakers: Anna Niarakis 01:15 - 01:30T (Replay) MEWpy: A Metabolic Engineering Workbench for Constraint-Based Strain Optimization Room 1 Speakers: Vítor Pereira 01:30 - 01:45T (Replay) Troppo, a Python Framework for Tissue-Specific Reconstruction and Phenotype Prediction Using **Omics Data** Room 1 Speakers: Vítor Vieira 01:45 - 02:00D Discussion Room 1 02:00 - 02:15B Break Room 1 T (Replay) VSM: the intuitive, general-purpose curation technology 02:15 - 02:30Room 1 Speakers: Steven Vercruysse 02:30 - 02:45Room 1 Speakers: Nicholas Roehner 02:45 - 03:00T (Replay) Modelling the Relationship between Design and Assembly Room 1 Speakers: Alexis Casas 03:00 - 03:15D Discussion Room 1 (Replay + Live Discussion) Information and data standards used at Ginkgo Bioworks Room 1 **PINNED** Speakers: Ariel Hecht 03:15 - 04:00S Social space/BREAK Room 1 **PINNED** 04:00 - 06:0006:00 - 06:15Room 1 Speakers: Isabel Marleen Pötzsch 06:15 - 06:30T (Replay) SABIO-RK: Curation and Visualization of Reaction Kinetics Data Room 1 Speakers: Ulrike Wittig 06:30 - 06:45T (Replay) EnzymeML – an SBML-based data exchange format for biocatalysis and enzymology Room 1 Speakers: Juergen Pleiss 06:45 - 07:00D Discussion Room 1 07:00 - 07:15B Break Room 1 07:15 - 07:30T (Replay) Stochastic Differential Equations and their Application in Systems Biology Room 1 Speakers: Stefan Hoops 07:30 - 07:45T (Replay) Towards in silico approaches for personalized medicine – Recommendations for verifying and validating predictive computational models in EU collaborative research Room 1 Speakers: Catherine Collin 07:45 - 08:00T (Replay) Automated Extraction of Implicit Molecular Structure from Reaction Network Models Room 1 Speakers: Ali Sinan Saglam 08:00 - 08:15D Discussion Room 1

| PINNED 08:15 – 09:00 | l (Replay + Live Discussion) TBA Speakers: Nathan Hillson | Room 1 |
|-----------------------------|---|--------------------|
| PINNED 09:00 – 10:00 | S Social space/BREAK | Room 1 |
| PINNED 10:00 – 10:45 | (Replay + Live Discussion) Putting energy into systems biology: biophysical models of cell systems understanding, simulation and design Speakers: Edmund Crampin | for Room 1 |
| 10:45 – 11:00 | T (Replay) A thermodynamic Model of EGFR and ERK Signaling explains Adaptive and Genetic Resistantesis Melanoma Speakers: Fabian Fröhlich | ance in Room 1 |
| 11:00 – 11:15 | T (Replay) The Systems Biology Graphical Notation: a standardised representation of biological maps Speakers: Michael Blinov | Room 1 |
| 11:15 – 11:30 | T (Replay) BioSimulators: a registry of containerized biosimulation tools with standard interfaces that the reuse of biomodels Speakers: Bilal Shaikh | enhance Room 1 |
| 11:30 – 11:45 | D Discussion | Room 1 |
| 11:45 – 12:00 | B Break | Room 1 |
| 12:00 – 12:15 | T (Replay) Datanator: an integrated database of molecular data for quantitatively modeling cellular bel Speakers: Lian Zhouyang | navior Room 1 |
| 12:15 – 12:30 | T (Replay) SBViper: Verification Testing of Kinetics Models in Systems Biology Speakers: Joseph L Hellerstein | Room 1 |
| 12:30 – 12:45 | T (Replay) pyPESTO: A python package for Parameter Estimation and Uncertainty Quantification Speakers: Jakob Vanhoefer | Room 1 |
| 12:45 – 13:00 | D Discussion | Room 1 |
| PINNED 13:00 – 14:00 | S Social space/BREAK | Room 1 |
| PINNED 14:00 – 14:45 | l (Replay + Live Discussion) CellDesigner: A modeling tool for biochemical networks Speakers: Akira Funahashi | Room 1 |
| 14:45 – 15:00 | T (Replay) A modular, thermodynamic approach for constructing large-scale kinetic models in system biology Speakers: Michael Pan | s Room 1 |
| 15:00 – 15:15 | T (Replay) Open Source and Sustainability Speakers: Jacob Barhak | Room 1 |
| 15:15 – 15:30 | T (Replay) Physiome - Make your model publications discoverable, reproducible, and reusable. Speakers: Karin Lundengård | Room 1 |
| 15:30 – 15:45 | D Discussion | Room 1 |
| 15:45 – 16:00 | B Break | Room 1 |
| 16:00 – 16:15 | T (Replay) OpenCOR: how to enable reproducible science using community standards and tools Speakers: Alan Garny | Room 1 |
| 16:15 – 16:30 | T (Replay) CellML 2.0 Speakers: David Nickerson | Room 1 |
| | | |
| 16:30 – 16:45 | T (Replay) Implementing OMEX metadata v1.1 Speakers: John Gennari | Room 1 |

| PINNED 17:00 – 18:00 | S Social space/BREAK | Room 1 |
|-----------------------------|--|-------------|
| PINNED 18:00 – 18:45 | l Reproducibility initiatives in computational biology Speakers: Jason Papin | Room 1 |
| 18:45 – 19:00 | T LibSBML 2020 and beyond Speakers: Sarah Keating | Room 1 |
| 19:00 – 19:15 | T pySBOL3: A Python library for SBOL 3 Speakers: Tom Mitchell | Room 1 |
| 19:15 – 19:30 | T Latest developments with the Python modeling package: Tellurium Speakers: Herbert Sauro | Room 1 |
| 19:30 – 19:45 | D Discussion | Room 1 |
| 19:45 – 20:00 | B Break | Room 1 |
| 20:00 – 20:15 | T Integration of sequence visualization into SynBioHub Speakers: Linhao Meng | Room 1 |
| 20:15 – 20:30 | T BpForms and BcForms: a toolkit for concretely describing non-canonical polymers and complexes to facilitate global biochemical networks Speakers: Paul F Lang | o Room 1 |
| 20:30 – 20:45 | T Quantitative study of spike propagation in a one-dimensional strand of detrusor smooth muscle cell Speakers: Chitaranjan Mahapatra | Room 1 |
| 20:45 – 21:00 | D Discussion | Room 1 |
| PINNED 21:00 – 21:45 | (Replay + Live Discussion) COVID-19 Disease Map: the key role of standards in community-driven development of systems biology disease models Speakers: Marek Ostaszewski | Room 1 |
| 21:45 – 22:00 | T (Replay) PEtab – Interoperable Specification of Parameter Estimation Problems in Systems Biology Speakers: Daniel Weindl | Room 1 |
| 22:00 – 22:15 | T (Replay) Spatial Model Editor Speakers: Liam Keegan | Room 1 |
| 22:15 – 22:30 | T (Replay) pyABC: likelihood-free inference Speakers: Emad Alamoodi | Room 1 |
| 22:30 – 22:45 | D Discussion | Room 1 |
| 22:45 – 23:00 | B Break | Room 1 |
| 23:00 – 23:15 | T (Replay) FAIRDOM: standard compliant data and model management Speakers: Olga Krebs | Room 1 |
| 23:15 – 23:30 | T (Replay) FAIR principles in literature-based kinetic modelling Speakers: Christoff Odendaal | Room 1 |
| 23:30 – 23:45 | T (Replay) Stochastic Modelling and Prediction of the COVID-19 Speakers: Joab Odhiambo | Room 1 |
| 23:45 – 00:00 | D Discussion | Room 1 |

R Breakout S Social space U Tutorial

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| OCTOBER 7 • WEDNESDA | <u> </u> | |
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| PINNED 00:00 – 01:00 | S Social space/BREAK | Room ⁻ |
| PINNED 04:00 – 06:00 | S Social space/BREAK | Room ⁻ |
| 06:00 - 09:00 | R SED-ML L1V4 Speakers: Matthias König | Room 1 |
| PINNED 09:00 – 10:00 | S Social space/BREAK | Room 1 |
| 10:00 – 12:00 | R Standards for curating flux balance constraint (FBC) models Speakers: Malik-Sheriff, Rahuman S. | Room 1 |
| 10:00 – 13:00 | R SBOL Libraries Roundtriping and Testing | Room SBOL |
| 12:00 – 13:00 | R What is the best way to add thermodynamic information to an SBML model? Speakers: Moritz Beber | Room 1 |
| PINNED 13:00 – 14:00 | S Social space/BREAK | Room 1 |
| 14:00 – 17:00 | R BioSimulations | Room 2 |
| 14:00 – 17:00 | R SBOL 3.0.1 | Room SBOL |
| 14:00 – 17:00 | R Towards in silico approaches for personalized medicine Speakers: Catherine Collin | Room 1 |
| PINNED 17:00 – 18:00 | S Social space/BREAK | Room 1 |
| 18:00 – 21:00 | R Systems Biology Graphical Notations Speakers: Michael Blinov | Room 2 |
| 18:00 – 21:00 | U Building, exploring and sharing rule-based models of cellular signaling pathways (I/II) Speakers: Martin Meier-Schellersheim | Room 1 |
| 18:00 – 21:00 | U SBOL Version 3: Simplified Data Exchange for Bioengineering Speakers: Jacob Beal | Room SBOL |
| 21:00 – 23:00 | R SBML Layout and Render Extensions Speakers: Herbert Sauro | Room 1 |

R Breakout S Social space U Tutorial

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| OCTO | DRFR 8 • | THURSDAY | | |

| PINNED 00:00 – 01:00 | S Social space/BREAK | Room 1 |
|-----------------------------|--|------------------------------|
| 01:00 - 03:00 | U Using Python HoloViz Technologies to Create Interactive Presentations Speakers: James Bednar, Jacob Barhak | Room 1 |
| PINNED 04:00 – 06:00 | S Social space/BREAK | Room 1 |
| 06:00 - 08:00 | U COPASI - an update on recently added functionality Speakers: Pedro Mendes | Room 1 |
| 08:00 - 09:00 | U Newt: view, design and analyze pathways in SBGN and more Speakers: Ugur Dogrusoz | Room 1 |
| PINNED 09:00 – 10:00 | S Social space/BREAK | Room 1 |
| 10:00 – 13:00 | R SBOL Validation Speakers: Christopher Myers | Room SBOL |
| 12:00 – 13:00 | R Discussion about centralizing data for calibrating and validating models and enabling stand Speakers: Jonathan Karr | dards (1/2) Room 1 |
| PINNED 13:00 – 14:00 | S Social space/BREAK | Room 1 |
| 14:00 – 17:00 | R Discussion about centralizing data for calibrating and validating models and enabling stand Speakers: Jonathan Karr | dards (2/2) Room 1 |
| 14:00 – 17:00 | R ELIXIR Systems Biology Focus Group Speakers: John Hancock | Room 2 |
| 14:00 – 17:00 | R SBOL Visual Parametric SVG Speakers: Christopher Myers | Room SBOL |
| PINNED 17:00 – 18:00 | S Social space/BREAK | Room 1 |
| 18:00 – 19:00 | U Equilibrator for Metabolic Network Analysis: Thermodynamic Profiling and Enzyme-Cost M Speakers: Moritz Beber | inimization Room 1 |
| 18:00 – 21:00 | U Building, exploring and sharing rule-based models of cellular signaling pathways (II/II) Speakers: Martin Meier-Schellersheim | Room 2 |
| 19:00 – 21:00 | U MAGINE: From time-series multi-omics to cellular mechanism of action Speakers: Alex Lubbock | Room 1 |
| 19:00 – 21:00 | U SBOL Visual: Communicating engineered biological designs with diagrams Speakers: Thomas Gorochowski | Room SBOL |
| 21:00 – 23:00 | R SED-ML Breakout Session Speakers: Herbert Sauro, Matthias König | Room 1 |
| 23:00 – 00:00 | R Model Annotation & the OMEX Metadata Spec v1.1 | Room 1 |

U Tutorial R Breakout **D** Discussion S Social space OCTOBER 9 · FRIDAY S Social space/BREAK Room 1 **PINNED** 00:00 - 01:0001:00 - 04:00U Center for Reproducible Biomedical Modeling Tutorial Room 1 Speakers: Veronica Porubsky S Social space/BREAK Room 1 **PINNED** 04:00 - 06:0006:00 - 09:00U libCelIML: How to get started Room 1 Speakers: Keri Moyle S Social space/BREAK Room 1 **PINNED** 09:00 - 10:0010:00 - 13:00R SBOL 3 Examples and Use Cases Room SBOL Speakers: Christopher Myers 11:00 - 13:00 R Reproducibility in Systems Biology Modelling Room 1 Speakers: Malik-Sheriff, Rahuman S. S Social space/BREAK Room 1 **PINNED** 13:00 - 14:0014:00 - 16:00R ModeleXchange - Are We Ready Yet? Room 1 Speakers: Henning Hermjakob 14:00 - 17:00R SBOL Visual Workflow and Ontology Room SBOL Speakers: Christopher Myers 14:00 - 17:00R Workshop on standardised neuronal network specifications Room 2 Speakers: Padraig Gleeson 16:00 - 17:00R Improving annotation and COMBINE archives: Problems, open research ideas & task brainstorming Room 1 Speakers: John Gennari S Social space/BREAK Room 1 PINNED 17:00 - 18:0018:00 - 19:00**U** FlapJack Room 1 Speakers: Gonzalo Vidal 18:00 - 19:00U PySB: a mathematical framework for modeling biochemical reactions as python programs Room 2 Speakers: Samantha Beik 19:00 - 21:00U Modelling with VCell Room 1 Speakers: Michael Blinov D Closing session Room 1 **PINNED** 21:00 - 21:30