

Day 1 (Feb 3 2022)

9h-9h30 **Intro:** *Setting the stage and objectives* by Valérie de Crécy-Lagard and Iddo Friedberg

9h30-12h **Session 1:** *Capture of what is known, past and future.*

Session co-chairs: Chris Mungall & Ana Conesa

Speakers:

9h30-9h40: Alan Bridge

9h40-9h50: Zhiyong Lu

9h50-10h00: Valerie Wood

10h00-10h10: Lucy Colwell

10h10-10h15: Elisha Wood-Charlson, Miro orientation

10h15-10h55 **Session1 Breakout Discussions**

Session1_Q1 -

What are major bottlenecks that face functional annotation resources to efficiently **collect** quality functional data? What actions could be proposed to address these bottlenecks?

Live Group 1 (Animator/Facilitator: Geoffrey Hutinet)

John Gerlt

Ana Conesa

Raquel Dias

Yousong Ding

Remote Group 1 (Animator/Facilitator: Anne Morgat)

Chris Henry

Gang Fang

Darren Natale

Francoise Thibaud-Nissen

Crysten Blaby-Haas

Chris Mungall

Cecilia Arighi

Iddo Friedberg

Alex Bateman

Valerie Wood

Katherine O'Toole

Session1_Q2

What are major bottlenecks that face functional annotation resources to accurately **describe** information on protein function? What actions could be proposed to address these bottlenecks?

Live Group 2 (Animator/Facilitator: Anita de Ward)

Valerie de Crecy-Lagard

Peter Uetz

Claire McWhite

Joshua Goldford

Richard Roberts

Remote Group 2 (Animator/Facilitator: Barbara Cheifet)

Adam Deutschbauer

Peter Weigle

Irina Rodionova

Gaurav D Moghe

Christine Orengo

Zhiyong Lu

Elisha Wood-Charlson

Maria-Jesus Martin

Christina MacLaughlin

David Vallenet

Alan James Bridge

Session1 _Q3

What are major bottlenecks that face functional annotation resources to accurately **share/transfer** information on protein function? What actions could be proposed to address these bottlenecks?

Live Group 3 (Animator/Facilitator: Seán O'Donoghue)

Christian Dallago

Benjamin Gyori

Gloria Sheynkman

Jeffrey Rudolf

Remote Group 3 (Animator/Facilitator: Stephen Burley)

Predrag Radivojac

Dmitri Rodionov

Lucy J. Colwell

Bill Nelson

Ian Blaby

Aron Marchler-Bauer

Antoine Danchin

Peter Karp

Lana Saleh

10h55-11h15 Coffee Break

11h15-12h **Session 1 wrap-up discussion** led by co-chairs Chris Mungall & Ana Conesa

12h00-13h00 Lunch break

13h00-15h30 **Session 2:** *What is an isofunctional family?*

Session co-chairs: John Gerlt, Paul Thomas & Alex Bateman

Speakers:

13h00-13h10 Intro to session by Alex Bateman (2mn) **and** John Gerlt (8mn),

13h10-13h20 Christine Orengo

13h20-13h30 Paul Thomas

13h30-13h40 Maria Martin

13h40-14h25 Session 2 Breakout Discussions

Session 2_Q1

What does it mean to be isofunctional? What constitutes adequate similarity in function to be isofunctional? Same reaction mechanism, same substrate specificity, same cellular pathways, same phenotypes, other?

Live Group 1 (Animator/Facilitator: Yousong Ding)

John Gerlt

Paul D. Thomas

Richard Roberts

Joshua Goldford

Raquel Dias

Remote Group 1 (Animator/Facilitator: Peter Weigele)

Chris Henry

Gang Fang

Lucy J. Colwell

Bill Nelson

Ian Blaby

Cecilia Arighi

Alex Bateman

Christina MacLaughlin

Antoine Danchin

Lana Saleh

Session2_Q2

What methods/tools can we use/develop to identify and create isofunctional families?

Live Group 2 (Animator/Facilitator: Jeffrey Rudolf)

Valerie de Crecy-Lagard

Claire McWhite

Christian Dallago

Benjamin Gyor

Geoffrey Hutinet

Remote Group 2 (Animator/Facilitator: Irina Rodionova)

Adam Deutschbauer

Darren Natale

Anne Morgat

Gaurav D Moghe

Christine Orengo

Zhiyong Lu

Maria-Jesus Martin
Iddo Friedberg
Stephen Burley
Peter Karp

Session2_Q3

How can different members of the community, both experimental and computational, collaborate on identifying and annotating isofunctional families, and make this information broadly available?

Live Group 3 (Animator/Facilitator: Peter Uetz)

Ana Conesa
Seán O'Donoghue
Anita de Waard
Gloria Sheynkman

Remote Group 3 (Animator/Facilitator: Aron Marchler-Bauer)

Predrag Radivojac
Dmitri Rodionov
Francoise Thibaud-Nissen
Alan James Bridge
Crysten Blaby-Haas
Chris Mungall
Elisha Wood-Charlson
Valerie Wood
David Vallenet
Barbara Cheifet
Katherine O'Toole

14h25-14h45 **Break**

14h45-15h30h **Session 2 wrap-up discussion** led by co-chairs John Gerlt, Paul Thomas & Alex Bateman

15h30-15h45 **Coffee Break**

15h45-18h00 **Session 3: *Mapping and propagating functional data to isofunctional group (Inference)***

Session co-chairs: Chris Henry & Gaurav Moghe

Speakers:

15h45-15h55 Gaurav Moghe
15h55-16h05 Francoise Thibaud-Nissen
16h05-16h15 Peter Karp
16h15h-16h25 Christian Dallago

16h25-17h05 **Session 3 Breakout Discussions**

Session3_Q1

How do we improve the accuracy of functional propagation? How do we evaluate accuracy?

Live Group 1 (Animator/Facilitator: Joshua Goldford)

Valerie de Crecy-Lagard
Richard Roberts
Paul D. Thomas
Christian Dallago
Yousong Ding

Remote Group 1 (Animator/Facilitator: Christine Orengo)

Adam Deutschbauer
Gang Fang
Irina Rodionova
Gaurav D Moghe
Ian Blaby
Cecilia Arighi
Alex Bateman
Christina MacLaughlin
Peter Karp
Antoine Danchin

Session3_Q2

How do we integrate, share, and credit functional information across resources?

Live Group 2 (Animator/Facilitator: Benjamin Gyori)

John Gerlt
Seán O'Donoghue
Anita de Waard
Jeffrey Rudolf
Geoffrey Hutinet

Remote Group 2 (Animator/Facilitator: Zhiyong Lu)

Peter Weigele
Darren Natale
Francoise Thibaud-Nissen
Alan James Bridge
Bill Nelson
Chris Mungall
Elisha Wood-Charlson
Iddo Friedberg
Stephen Burley
Lana Saleh

Session3_Q3

How can automated computer algorithms help (e.g. modeling, machine learning)?

Live Group 3 (Animator/Facilitator: Raquel Dias)

Ana Conesa
John Gerlt
Claire McWhite

Gloria Sheynkman
Peter Uetz

Remote Group 3 (Animator/Facilitator: Dmitry Rodionov)

Predrag Radivojac
Lucy J. Colwell
Anne Morgat
Chris Henry
Crysten Blaby-Haas
Aron Marchler-Bauer
Maria-Jesus Martin
Valerie Wood
David Vallenet
Barbara Cheifet
Katherine O'Toole

17h05-17h20 **Break**

17h20-18h00 **Session 3 wrap-up discussion** led by co-chairs Chris Henry & Gaurav Moghe

18h30 Dinner with talk EVENING SPEAKER at 19h00 : Dr Drew Berry

Day 2 Feb4 2022

8h30 -10h45 **Session 4:** *Building a new data-driven biological culture: challenges in training and culture changes to create data that is FAIR and machine readable.*

Session co-chairs: Elisha Wood-Charlson & Ian Blaby

Speakers:

8h30-8h40 Elisha Wood-Charlson
8h40-8h50 Geoffrey Hutinet
8h50-9h00 Steven Burley
9h00-9h10 Benjamin Gyori

9h10-09h50 **Session 4 Breakout Discussions**

Session4_Q1

What are the current challenges impeding data discovery and access from either online resources or the published literature?

Live Group 1 (Animator/Facilitator: Gloria Sheynkman)

Peter Uetz
Benjamin Gyori
Raquel Dias
Jeffrey Rudolf
Geoffrey Hutinet

Remote Group 1 (Animator/Facilitator: Predrag Radivojac)

Peter Weigele
Irina Rodionova
Alan James Bridge
Gaurav D Moghe
Bill Nelson
Zhiyong Lu
Elisha Wood-Charlson
Lana Saleh
Christina MacLaughlin
Antoine Danchin

Session4_Q2 -

How can annotation data be made more machine-readable?

Live Group 2 (Animator/Facilitator: Ana Conesa)

John Gerlt
Claire McWhite
Paul D. Thomas
Joshua Goldford
Richard Roberts

Remote Group 2 (Animator/Facilitator: Adam Deustchbauer)

Chris Henry
Dmitri Rodionov
Darren Natale
Francoise Thibaud-Nissen
Crysten Blaby-Haas
Chris Mungall
Maria-Jesus Martin
Alex Bateman
Stephen Burley
Peter Karp

Session4_Q3

How can annotation data be made more approachable and accessible to all users, and how can users trust the veracity of deposited data?

Live Group 3 (Animator/Facilitator: Christian Dallago)

Valerie de Crecy-Lagard
John Gerlt
Seán O'Donoghue
Anita de Waard
Yousong Ding

Remote Group 3 (Animator/Facilitator: Valerie Wood)

Gang Fang
Lucy J. Colwell
Anne Morgat
Christine Orengo

Ian Blaby
Aron Marchler-Bauer
Cecilia Arighi
Iddo Friedberg
David Vallenet
Barbara Cheifet
Katherine O'Toole

09h50-10h05 **Break**

10h05-10h45 **Session 4 wrap-up discussion** led by co-chairs Elisha Wood-Charlson & Ian Blaby

10h45-11h00 **Break**

11h00-13h00 **Session 5:** *Automation of functional data generation: challenges in designing, conducting and capturing high-throughput functional screening assays to increase functional knowledge at the pace of the potential of computational methods to process and propagate this knowledge.*

Session co-chairs: Adam Deutschbauer & Iddo Friedberg

Speakers:

11h00-11h10 Crysten Blaby-Haas
11h10-11h20 Irina Rodionova
11h20-11h30 Gloria Sheynkman
11h30-11h40 Peter Uetz

11h40-12h15 **Session 5 Breakout Discussions**

Session5_Q1

What's the value and best usage of high-throughput "functional" data (beyond just sequence data) for functional annotation of proteins?

Live Group 1 (Animator/Facilitator: Claire McWhite)

John Gerlt
Paul D. Thomas
Benjamin Gyori
Jeffrey Rudolf

Remote Group 1 (Animator/Facilitator: Francoise Thibaud-Nissen)

Adam Deutschbauer
Peter Weigele
Anne Morgat
Gaurav D Moghe
Christine Orengo
Cristen Blaby-Haas
Aron Marchler-Bauer
Maria-Jesus Martin
Christina MacLaughlin
Barbara Cheifet

Session5_Q2

What data types are most critical, and can these data be generated at scale for diverse organisms/protein families?

Live Group 2 (Animator/Facilitator: Joshua Goldford)

Valerie de Crecy-Lagard
Seán O'Donoghue
Richard Roberts
Raquel Dias

Remote Group 2 (Animator/Facilitator: Bill Nelson)

Chris Henry
Gang Fang
Darren Natale
Francoise Thibaud-Nissen
Irina Rodionova
Ian Blaby
Chris Mungall
Cecilia Arighi
Iddo Friedberg
David Vallenet
Katherine O'Toole

Session5_Q3

How can data from HT experiments be incorporated into annotations within established databases?

Live Group 3 (Animator/Facilitator: Christian Dallago)

Ana Conesa
Anita de Waard
Gloria Sheynkman
Yousong Ding
Geoffrey Hutinet

Remote Group 3 (Animator/Facilitator: Peter Karp)

Predrag Radivojac
Dmitri Rodionov
Lucy J. Colwell
Alan James Bridge
Bill Nelson
Zhiyong Lu
Elisha Wood-Charlson
Valerie Wood
Alex Bateman
Stephen Burley
Lana Saleh

12h15-12h30 **Break**

12h30-13h00 **Session 5 wrap-up discussion** led by co-chairs Adam Deutschbauer & Iddo Friedberg

13h00-14h30 **Session 6 with lunch** *Synthesis, creating the roadmap for efficient and accurate functional annotation of the global proteome.* (talks 35 mn, discussion 40 mn, closing 15mn by Valérie de Crécy-Lagard)

Session co-chairs: Sean O'Donoghue & Valérie de Crécy-Lagard

Speakers :

13h00-13h15 Sean O'Donoghue

13h15-13h25 Chris Mungall

13h25-13h35 Rich Roberts

13h35-14h20 **Session 6 whole group discussion** led by Rich Roberts & Chris Mungall

Session6_Q1

How can communication and collaboration between the biocurators and experimentalist communities be improved?

Session6_Q2

What funding mechanisms and incentives could be used to move the field forward?

14h20-14h30 Closing meeting **Valérie de Crécy-Lagard**