Agenda for EMDataResource Ligand Challenge Wrap Up Meeting

July 26-28 11 AM start, length varies 2-4 hrs per day.

All times noted are US Eastern (New York)

Time Conversion: US PT -3 / US CT -1 / UK +5 / EUR +6

Ligand Challenge Links

Main Challenge Info Page: https://challenges.emdataresource.org/?q=2021-model-challenge

Model Compare Analysis: https://model-compare.emdataresource.org

Possibly Helpful Guides from Previous Challenges

Guidance for Modeler/Assessor Presentations - pdf - (2017)

Guidance for Challenge Discussion - pdf - (2019)

Zoom Connection Information

Topic: Ligand Challenge Wrap Up 3 Day Meeting

Time: Jul 26, 2021 11:00 AM Eastern Time (US and Canada)

Every day, 3 occurrence(s)

Jul 26, 2021 10:30 AM Open for testing, Casual Discussion 11 AM - 3 PM Presentations

Jul 27, 2021 10:30 AM Open for testing, Casual Discussion 11 AM - 2 PM: Presentations

Jul 28, 2021 10:30 AM Open for testing, Casual Discussion 11 AM - 1 PM Discussion

iCalendar (.ics) files to your calendar system:

https://rutgers.zoom.us/meeting/tJ0sduquqj8qGNbE688-39kN-Ndo0ODFuZ53/ics?icsToken=98tyKuChrzopHNCRsBuFRox5BYj4b-7wiClfjY1fuUm9W20AOwjYe8xGPeJQNP7F

Join Zoom Meeting

https://rutgers.zoom.us/j/99113644022?pwd=dGY5LzhGaGlZU2lhb3Z0aWFHNExKUT09

Join by SIP: 99113644022@zoomcrc.com

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Find your local number: https://rutgers.zoom.us/u/adl8iC4lAx

Join by Skype for Business: https://rutgers.zoom.us/skype/99113644022

If you have any questions, please contact the Office of Information Technology Help Desk: https://it.rutgers.edu/help-support/

Day 1: presentations by each submitting team (July 26th; 4 hours)

10:30 - 11:00 (US Eastern) Zoom call opens early for presenter checks, casual discussion

11:00 - 11:10 Welcome, Short Introduction Cathy Lawson/Wah Chiu

11:04 - 15:00 Presentations (10 Minutes per Team plus 4 minutes discussion)

Introduce Team, Summarize methods used, identify any challenges faced, particularly with regards to ligand modeling.

Session I

Chair: Cathy Lawson

Team Members/Presenters	Talk Title	Start Time
Colin Palmer, Rob Nicholls, Rangana Warshamanage, Keitaro Yamashita, Garib Murshudov, Paul Bond, Scott Hoh, Mateusz Olek, Kevin Cowtan, Agnel Joseph, Tom Burnley, Martyn Winn	Utilizing Tools in CCP-EM for Model Refinement and Validation	11:10
Dong Si, Sean Lin, Minglei Zhao, Renzhi Cao, Jie Hou	DeepTracer Team 2021 Ligand Model Challenge Summary	11:24
Grzegorz Chojnowski	Modelling the Ligand Challenge targets de novo	11:38
Daisuke Kihara, Genki Terashi, Daipayan Sarkar, Jacob Verburgt	Ligand modeling by Kiharalab	11:52
Abishek Singharoy, Sumit Mittal, Alberto Perez, Daisuke Kihara, Mrinal Shekhar, Daipayan Sarkar, Genki Terashi, Chris Rowley, Reza Esmaeli, Lijun Lang, Arup Mondal, Arthur Campbell	CryoFold Modelling for EMDR Ligand Challenge	12:06
Gunnar Schröder, Luisa Schäfer, Karunakar R. Pothula	Cross-validation approach to fit small molecules into cryo-EM maps	12:20
Andrew Muenks, Frank DiMaio	Density-guided modeling of small molecules and ions with Rosetta	12:34

12 minute break	12:48-13:00

Session II

Chair Andriy Kryshtafovych

Team Members/Presenters	Talk Title	Start Time
Wei-Chun Kao	Modeling alternate ligand conformation	13:00
Alberto Perez, Arup Mondal, Reza Esmaeli, Lijun Lang	Extracting Water densities from MD	13:14
Nigel Moriarty, Pavel Afonine, Christopher Schlicksup, Oleg Sobolev	Recent Developments in Phenix for Cryo-EM Model Refinement	13:28
Jianlin Cheng, Nabin Giri	Structure Determination from cryo-EM Density Maps Using a Deep Learning Framework	13:42
Simone Weyand, Sundeep Chaitanya, Tom Blundell, Steven Brohawn	TBD	13:56
Dilip Kumar	Automated or Manual intervention: striking the right balance	14:10
Matthew Baker, Corey Hryc	Beyond Pathwalker: Modeling Ligands in CryoEM Density Maps	14:24
Greg Pintilie, Michael Schmid, Wah Chiu	Modeling ligands, water, ions in CryoEM maps with SegMod and SWIM	14:38

Discussion	14:52-15:00

Modeler group not presenting: Helmut Grubmuller

Day 2: presentations by each assessor group (July 27th; 3 hours)

10:30 - 11:00 (US Eastern) Zoom call opens early for presenter checks, casual discussion

11:00 - 11:10 Welcome, Short Introduction Cathy Lawson/Wah Chiu

11:10 - 14:00 Presentations (20 Minutes per Team, including 4 minutes discussion)

Introduce Team, Summarize methods used, identify any challenges faced, particularly with regards to ligand model assessments

Chairs: Helen Berman / Mike Schmid

Assessor Team/Presenter	**Talk Title**	**Start Time**
Andriy Kryshtafovych	Model Compare Pipeline Trends	11:10
Chenghua Shao	Validation of ligands at the wwPDB	11:30
Paul Emsley	Validating Models using Coot Tools	11:50
Bohdan Schneider, Jiří Černý	Nucleic acid conformations / Protein hydration analysis	12:10
10 Minute Break		12:30
Jane Richardson, Christopher J. Williams, Vincent Chen, David Richardson	Ligands, ions, & waters assessed by contact analysis, partial occupancy, & visual examination	12:40
Chris I. Williams, Chemical Computing Group Support Team	Using Consensus Pharmacophore Fields to Score Placed Fragments	13:00
Ben Sellers, Alberto Gobbi, Alexis Rohou	Assessment of internal strain energy in ligand models	13:20
Greg Pintilie, Michael Schmid, Wah Chiu	Assessment of water, ions and ligands in CryoEM maps with Q-scores	13:40

Day 3: Wrap up discussion (July 28th; 2 hours)

Chair: Cathy Lawson

10:30 - 11:00 (US Eastern) Zoom call opens early for casual discussion

11:00 - 11:10 Short Intro Cathy Lawson

11:10 - 11:40 Discussion: Challenge outcomes: Modellers' perspectives

11:40 - 12:10 Discussion: Challenge outcomes: Assessors' perspectives

Jane Richardson: Ensembles win, occupancy matters, ions need tools, and other stories

12:10 - 12:40 Discussion: Key Outcomes

12:40 - 13:00 Discussion: What's Next

Participants

All invitees

Pavel	Afonine	pafonine@lbl.gov	Lawrence Berkeley Laboratory
Matthew L	Baker	Matthew.L.Baker@uth.tmc.edu	University of Texas Houston
Helen	Berman	hmbmay19@gmail.com	Rutgers University (Emerita)
Paul	Bond	paul.bond@york.ac.uk	York University
Stephen	Burley	stephen.burley@rcsb.org	Rutgers University
Arthur	Campbell	arthurc@broadinstitute.org	Broad Institute
Renzhi	Cao	caora@plu.edu	Pacific Lutheran University
Jiří	Černý	jiri.cerny@ibt.cas.cz	Czech Academy of Sciences
Sundeep	Chaitanya	scv26@cam.ac.uk	University of Cambridge
Vincent	Chen	vbchen@gmail.com	Duke University
Jianlin	Cheng	chengji@missouri.edu	University of Missouri
Chih-Ta	Chien	ctc40@stanford.edu	Stanford University
Wah	Chiu	wahc@stanford.edu	Stanford University
Grzegorz	Chojnowski	gchojnowski@embl-hamburg.de	EMBL Hamburg
Frank	DiMaio	dimaio@uw.edu	University of Washington
Alison	Doerr	a.doerr@us.nature.com	Nature Methods (Journal)
Paul	Emsley	pemsley@mrc-lmb.cam.ac.uk	MRC-LMB Cambridge
Reza	Esmaeli	reza.esmaeeli@chem.ufl.edu	University of Florida
Paula	Flicker	flickerp@nigms.nih.gov	NIH/NIGMS
Michael	Funk	mfunk@aaas.org	Science (Journal)
Nabin	Giri	ngzvh@missouri.edu	University of Missouri
Helmut	Grubmuller	hgrubmu@gwdg.de	Max Planck Institute Göttingen
Mark	Herzik	mherzik@ucsd.edu	University of California San Diego
Scott	Hoh	soonwen.hoh@york.ac.uk	University of York
Jie	Hou	jie.hou@slu.edu	Saint Louis University
Corey	Hyrc	Corey.F.Hryc@uth.tmc.edu	University of Texas Houston
Maxim	Igaev	migaev@mpibpc.mpg.de	Max Planck Institute Göttingen
Andrzej	Joachimiak	andrzejj@anl.gov	Argonne National Laboratory
Agnel	Joseph	agnel-praveen.joseph@stfc.ac.uk	UKRI Science Technology Facilities Council
Wei-Chun	Kao	wei-chun.kao@biochemie.uni-freiburg.de	University of Freiburg
Daisuke	Kihara	dkihara@purdue.edu	Purdue University
Rachael	Kretsch	rkretsch@stanford.edu	Stanford University
Andriy	Kryshtafovych	akryshtafovych@ucdavis.edu	University of California Davis
Karin	Kuehnel	Karin.Kuehnel@nature.com	Nature Communications (Journal)
Lijun	Lang	lijunlang@chem.ufl.edu	University of Florida
Cathy	Lawson	cathy.lawson@rcsb.org	Rutgers University
Sean	Lin	chlin19@uw.edu	University of Washington
Sumit	Mittal	smitta25@asu.edu	Arizona State University
Arup	Mondal	arup.mondal@chem.ufl.edu	University of Florida
Andrew	Muenks	amuenks@uw.edu	University of Washington
Sigrid	Noreng	norengs@gene.com	Genentech
Nigel	Moriarty	nwmoriarty@lbl.gov	Lawrence Berkeley Laboratory
Mateusz	Olek	mateusz.olek@diamond.ac.uk	Diamond Light Source
Colin	Palmer	colin.palmer@stfc.ac.uk	UKRI Science Technology Facilities Council
Sushrit	Pasumarthy	sushritp1@gmail.com	Duke University
Alberto	Perez	perez@chem.ufl.edu	University of Florida
Grigore	Pintilie	gregdp@stanford.edu	Stanford University
Emmi	Pohjolainen	emmi.pohjolainen@mpibpc.mpg.de	Max Planck Institute Göttingen

Joann	Polizzi	joannp@stanford.edu	Stanford University
Karunakar	Pothula	k.pothula@fz-juelich.de	Forschungszentrum Jülich
Michael	Prisant	michael.prisant@gmail.com	Duke University
Randy	Read	rjr27@cam.ac.uk	University of Cambridge
Dave	Richardson	dcr@kinemage.biochem.duke.edu	Duke University
Jane	Richardson	jsr@kinemage.biochem.duke.edu	Duke University
Alexis	Rohou	rohoua@gene.com	Genentech
Chris	Rowley	cnrowley@gmail.com	Arizona State University
Daipayan	Sarkar	dsarkar@asu.edu	Arizona State University
Luisa	Schäfer	lu.schaefer@fz-juelich.de	Forschungszentrum Jülich
Christopher	Schlicksup	cjschlicksup@lbl.gov	Lawrence Berkeley Laboratory
Michael	Schmid	mfschmid@stanford.edu	Stanford University
Bohdan	Schneider	bohdan.schneider@gmail.com	Czech Academy of Sciences
Gunnar	Schröder	gu.schroeder@fz-juelich.de	Forschungszentrum Jülich
Ben	Sellers	sellers.benjamin@gene.com	Genentech
Chenghua	Shao	chenghua.shao@rcsb.org	Rutgers University
Mrinal	Shekhar	mshekhar@broadinstitute.org	Broad Institute
Dong	Si	dongsi@uw.edu	University of Washington
Abhishek	Singharoy	asinghar@asu.edu	Arizona State University
Oleg	Sobolev	osobolev@lbl.gov	Lawrence Berkeley Laboratory
Elizabeth	Sourial	esourial@chemcomp.com	Chemical Computing Group
Guan Chin	Su	gcsu@stanford.edu	Stanford University
Sai	Subramaniya	smaddhur@purdue.edu	Purdue University
Genki	Terashi	gterashi@purdue.edu	Purdue University
Andrea	Vaiana	avaiana@mpibpc.mpg.de	Max Planck Institute Göttingen
Brinda	Vallat	brinda.vallat@rcsb.org	Rutgers University
Xiao	Wang	wang3702@purdue.edu	Purdue University
Simone	Weyand	sw644@cam.ac.uk	University of Cambridge
Chris I	Williams	cwilliams@chemcomp.com	Chemical Computing Group
Christopher J	Williams	christopher.sci.williams@gmail.com	Duke University
Mary Ann	Wu	maryann.wu@nih.gov	NIH/NIGMS
Keitaro	Yamashita	kyamashita@mrc-lmb.cam.ac.uk	MRC-LMB Cambridge
Minglei	Zhao	mlzhao@uchicago.edu	University of Chicago

Advisors
Bohdan Schneider, Paul Emsley, Jiří Černý, Alexis Rohou, Andrzej Joachimiak, Randy Read, Jane Richardson

EMDR
Wah Chiu, Cathy Lawson, Helen Berman, Michael Schmid, Andriy Kryshtafovych, Greg Pintilie

Modeling Team Leads
Dilip Kumar, Dong Si, Daisuke Kihara, Abhishek Singharoy, Andrew Muenks, Grzegorz Chojnowski, We-Chun Kao, Alberto Perez, Nigel Moriarty, Greg Pintilie, Simon Weyand, Colin Palmer, Matthew Baker, Paul Emsley, Gunnar Schroeder, Helmut Grubmuller, Jianlin Cheng

Assessor Team Leads
Bohdan Schneider, Jiří Černý,Chenghua Shao, Andriy Kryshtafovych,Elizabeth Sourial, Alexis Rohou, Mark Herzik,Jane Richardson,Ben Sellers, Paul Emsley