

Agenda for EMDataResource Ligand Challenge Wrap Up Meeting

July 26-28 11 AM start, length varies 2-3.75 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](#)

[Possibly Helpful Guides from Previous Challenges](#)

[Zoom Connection Information](#)

[Day 1: presentations by each submitting team \(July 26th; 3.75 hours\)](#)

[Session I](#)

[Session II](#)

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

[Day 3: Wrap up discussion \(July 28th; 2 hours\)](#)

[Email lists](#)

[Advisors](#)

[EMDR](#)

[Modeling Team Leads](#)

[Assessor Team Leads](#)

[All invitees](#)

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 - 2:45 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=dGY5LzhGaGIZU2lhb3Z0aWFHNExKUT09>

Join by SIP: 99113644022@zoomcrc.com

Meeting ID: 991 1364 4022

Password: 251406

One tap mobile

+13126266799,,99113644022# US (Chicago)

+16465588656,,99113644022# US (New York)

Join By Phone

+1 312 626 6799 US (Chicago)

+1 646 558 8656 US (New York)

+1 301 715 8592 US (Washington DC)

+1 346 248 7799 US (Houston)

+1 669 900 9128 US (San Jose)

+1 253 215 8782 US (Tacoma)

Meeting ID: 991 1364 4022

Find your local number: <https://rutgers.zoom.us/u/adl8iC4IAx>

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; 3.75 hours)

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

11:00 - 11:04 Welcome, Short Introduction Cathy Lawson/Wah Chiu

11:04 - 14:45 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

Team Members/Presenters	Talk Title	Start Time
<u>Colin Palmer</u> , 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	11:04
<u>Dong Si</u> , <u>Sean Lin</u> , Minglei Zhao, Renzhi Cao, Jie Hou	DeepTracer Team 2021 Ligand Model Challenge Summary	11:18
<u>Grzegorz Chojnowski</u>	Modelling the Ligand Challenge targets de novo	11:32
<u>Daisuke Kihara</u> , Genki Terashi, Daipayan Sarkar, Jacob Verburgt	Ligand modeling by Kiharalab	11:46
<u>Abishek Singharoy</u> , Sumit Mittal, Alberto Perez, Daisuke Kihara, <u>Mrinal Shekhar</u> , <u>Daipayan Sarkar</u> , Genki Terashi, Chris Rowley, Reza Esmaeli, Lijun Lang, Arup Mondal, Arthur Campbell	CryoFold Modelling for EMDR Ligand Challenge	12:00
Gunnar Schröder, Luisa Schäfer, <u>Karunakar R. Pothula</u>	Cross-validation approach to fit small molecules into cryo-EM maps	12:14
<u>Andrew Muenks</u> , Frank DiMaio	Density-guided modeling of small molecules and ions with Rosetta	12:28
8 minute break		12:42

Session II

Team Members/Presenters	Talk Title	Start Time
<u>Wei-Chun Kao</u>	Modeling alternate ligand conformation	12:50
<u>Alberto Perez</u> , Arup Mondal, Reza Esmaeli, Lijun Lang	Extracting Water densities from MD	13:04
Nigel Moriarty, Pavel Afonine, <u>Christopher Schlicksup</u> , Oleg Sobolev	Recent Developments in Phenix for Cryo-EM Model Refinement	13:18
Jianlin Cheng, <u>Nabin Giri</u>	Structure Determination from cryo-EM Density Maps Using a Deep Learning Framework	13:32
Simone Weyand, <u>Sundeeep Chaitanya</u> , Tom Blundell, Steven Brohawn	TBD	13:46
<u>Dilip Kumar</u>	Automated or Manual intervention: striking the right balance	14:00
<u>Matthew Baker</u> , Corey Hryc	Beyond Pathwalker: Modeling Ligands in CryoEM Density Maps	14:14
<u>Greg Pintilie</u> , Michael Schmid, Wah Chiu	Modeling ligands, water, ions in CryoEM maps with SegMod and SWIM	14:28

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

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

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

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

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

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EMDR

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