Agenda

Sightseeing Saturday

See our favorite sightseeing options WinterRosettaCon 2018/Sightseeing

Saturday

Hotel check-in after 3 pm

- 7:30 pm Meet people at TODO for dinner and drinks

Sunday

- 08:00 Breakfast at GDFA
- 08:50 Welcome and Code of conduct [PDF (https://www.dropbox.com/s/9z6so9c26t0o0hm/renfrew-introduction.pdf?dl=0)]

09:00 – 10:20 Session I: Membranes, Session Chair: TBD

- 09:00 – 09:20 **TBD**: *Introduction and Diversity and Inclusion Committee*
- 09:20 – 09:40 **Alican Gulsevin**: *Prediction of amphipathic helix - membrane interactions with Rosetta*
- 09:40 – 10:00 **Rebecca Alford**: *Diverse scientific benchmarks reveal optimization imperatives for implicit membrane energy functions*
- 10:00 – 10:20 **Bobby Langan**: *Rapid design of transmembrane domains on a distributed computing system*

10:20 – 10:40 Break

Coffee and snacks on the GDFA promenade

10:40 – 12:00 Session II: Incorporating Experimental Data, Session Chair: Elleansar Okwei

- 10:40 – 11:00 **Sarah Biehn**: *Improving Rosetta protein structure prediction with hydroxyl radical footprinting mass spectrometry data*
- 11:00 – 11:20 **Justin Seffernick**: *Using Data from Surface-Induced Dissociation (SID) to Predict Structures of Protein Complexes and Vice Versa*
- 11:20 – 11:40 **Daniel Marzolf**: *Computational Analysis of NMR-determined Hydrogen-Deuterium Exchange Rates via de novo Structure Prediction*
- 11:40 – 12:00 **Kevin Drew**: *Identifying direct protein interactions through high throughput proteomics*

12:00 – 01:00 Lunch

The midday meal will be served on the GDFA promenade. We have a few lunch tables, you can check out the assignments here (https://docs.google.com/spreadsheets/d/17RktMG7XXnDo5sS-9j5GlN8OIszhO_N3m19rnLBgrKo/edit?usp=sharing)

01:00 – 02:20 Session III: Development I, Session Chair: Maria Szegedy

- 01:00 – 01:20 **Sergey Lyskov**: *Benchmark Server, the essentials*
- 01:20 – 01:40 **Andrew Leaver-Fay**: *Tmol Update*

- 01:40 – 02:00 **Jason Labonte**: *EnzymaticMovers: A Framework for Post-Translational Modifications in Rosetta*
- 02:00 – 02:20 **Teun Hoevenaars**: *Preliminary Results of Jacobi Refinement Mover*

02:20 – 03:50 Breakout Session in parallel with Rosetta101 and Intern meeting, Session Chair: Julia & Doug

- 02:20 – 03:50 Rosetta101 in the 162 2nd floor auditorium
- 02:20 – 03:50 Intern meeting at 162 8th floor conference room. Chair: Jeff Gray
- 02:20 – 03:05 Breakout Session I - please pick session here (https://docs.google.com/spreadsheets/d/17RktMG7XXnDo5sS-9j5GlN8OIszhO_N3m19rnLBgrKo/edit?usp=sharing)
- 03:05 – 03:50 Breakout Session II - please pick session here (https://docs.google.com/spreadsheets/d/17RktMG7XXnDo5sS-9j5GlN8OIszhO_N3m19rnLBgrKo/edit?usp=sharing)

04:00 – 04:20 Break

Coffee and snacks will be served on the GDFA promenade.

04:20 – 05:20 Session IV: Design I, Session Chair: Brian Weitzner

- 04:20 – 04:40 **Alena Khmelinskaia**: *Breaking the symmetry of protein assemblies: structural flexibility as a de novo design principle*
- 04:40 – 05:00 **Ajasja Ljubetic**: *First steps towards a de-novo designed random protein walker*
- 05:00 – 05:20 **Elif Nihal Korkmaz**: *Towards designing better de novo peptide binders*

05:20 – 06:00 Keynote I: Session Chair: Helen Ji

- **Liz Kellogg**: *Computation and Cryo-EM: a vision for the future of structural biology*

06:00 – 07:00 Diner I, Location: Flatiron Institute Cafeteria

We will cross the street to the top of the Flatiron Institute for diner and the view.

07:00 – 09:00 Poster Session I - First names A - J, Location: GDFA Promenade

Posters will be accompanied by dessert and drinks.

Monday

- 8:00 Breakfast at GDFA

09:00 – 10:20 Session V: Design II, Session Chair: Jing Zhou

- 09:00 – 09:20 **Jack Maguire**: *What was wrong with FastDesign and how can we prevent these problems in future protocols?*
- 09:20 – 09:40 **Brian Kuhlman**: *Stabilizing proteins with Rosetta*
- 09:40 – 10:00 **Marion Sauer**: *RECON multi-state design predicts sequences optimal for conformational change*
- 10:00 – 10:20 **Colin Smith**: *Dynamics and Stability of de novo Designed Mini-Proteins*

10:20 – 10:40 Break

Coffee and snacks on the GDFA promenade

10:40 – 12:00 Session VI: Antibodies, Session Chair: Raulia Syrlybaeva

- 10:40 – 11:00 **Roland Dunbrack**: *Structural classification of antibody CDRs for computational design*
- 11:00 – 11:20 **Clara Schoeder**: *Structure-based vaccine design to elicit broadly neutralizing antibodies for Filoviruses*
- 11:20 – 11:40 **Jeliazko Jeliazkov**: *Robustifying Rosetta Antibody*
- 11:40 – 12:00 **Odessa Goudy**: *Designing safer cancer immunotherapies: Autoinhibited PD-1 decoys*

12:00 – 01:00 Lunch

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01:00 – 02:20 Session VII: Specialized applications, Session Chair: Justyna Kryś

- 01:00 – 01:20 **AJ Vincelli**: *A Consensus Method of Relaxing Protein X-Ray Structural Models To Improve Their Quality Scores*
- 01:20 – 01:40 **Adam Moyer**: *Computational Discovery of Polypeptide Secondary Structures from Synthetic Amino Acids*
- 01:40 – 02:00 **James Baggs Eastwood**: *Designing peptoid macrocycles to bind protein surfaces*
- 02:00 – 02:20 **Aleksandra Badaczewska-Dawid**: *Multiscale protein-peptide docking using CABS-dock and FlexPepDock*

02:20 – 04:00 Discussion Session, Session Chair: Andrew Leaver-Fay

Discussion topics are towards the end of this page.

04:00 – 04:20 Break

Coffee and Cronuts from Dominique Ansel Bakery; February's flavor is strawberry jam and honey walnut ganache.

04:20 – 05:20 Session VIII: Machine Learning, Session Chair: Ryan Feehan

- 04:20 – 04:40 **Vikram Mulligan**: *Neural networks and quantum computers: New technologies for peptide and protein design*
- 04:40 – 05:00 **Jeffrey Gray**: *Can Deep Learning Give Us Sub-Angstrom Accuracy on Antibody Loops?*
- 05:00 – 05:20 **Brandon Frenz**: *Determining the structure of the coronavirus spike glycan shield using CryoEM and Rosetta*

05:20 – 06:00 Keynote II: Session Chair: Bridger Woods

- **James Moody**: *Protein crystallization facilitated by protein polymers*

06:00 – 07:00 Diner II, Location: Flatiron Institute Cafeteria

We will cross the street to the top of the Flatiron Institute for diner and the view.

07:00 – 09:00 Poster Session II - First names K - Z, Location: GDFA Promenade

Posters will be accompanied by dessert and drinks.

Tuesday

- 8:00 Breakfast at GDFA

09:00 – 10:20 Session IX: Design III, Session Chair: Daniel Berenberg

- 09:00 – 09:20 **Matthew O'Meara**: *Designer proteins for nerve regeneration*
- 09:20 – 09:40 **Frank Teets**: *Hyperspatial de novo design*
- 09:40 – 10:00 **Summer Thyme**: *Using Rosetta for Problems in Neurodevelopmental Disease and Precision Medicine*
- 10:00 – 10:20 **Will Hansen**: *Photoswitchable and multinuclear metal binding by design*

10:20 – 10:40 Break

Coffee and snacks on the GDFA promenade

10:40 – 12:00 Session X: Meta, Session Chair: TBD

- 10:40 – 11:00 **Sam DeLuca**: *A better world is possible: patterns for reproducible computational science*
- 11:00 – 11:20 **Ashley Vater**: *Using Foldit and benchmarking in the classroom*
- 11:20 – 11:40 **Andrew Watkins**: *Nonprofit organization to facilitate direct mutual aid among Rosetta trainees*
- 11:40 – 12:00 **Karen Khar**: *Diversity training proposal*

12:00 – 01:00 Lunch

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01:00 – 02:20 Session XI: Development/PyRosetta, Session Chair: Daniel Zaidman

- 01:00 – 01:20 **Rocco Moretti**: *Rosetta Drug Developement*
- 01:20 – 01:40 **Kathy Le**: *Multimedia Jupyter Notebooks for Learning Biomolecular Structure Prediction and Design*
- 01:40 – 02:00 **Justyna Krys**: *PyRosetta Web Application*
- 02:00 – 02:20 **Joanna Macnar**: *PyRosetta web application for small ligand - protein docking*

02:20 – 03:50 Breakout Session, Session Chair: TBD

- 02:20 – 03:20 Breakout session III - please pick session here (https://docs.google.com/spreadsheets/d/17RktMG7XXnDo5sS-9j5GlN8OIszhO_N3m19rnLBgrKo/edit?usp=sharing)
- 03:20 – 03:50 **TBD**: *Breakout session summaries*

04:00 – 04:20 Break

Coffee and snacks on the GDFA promenade

04:20 – 05:20 Session XII: Enzymes & Folding, Session Chair: Jaden Anderson

- 04:20 – 04:40 **Sina Kordes**: *Extending a de novo designed TIM barrel*
- 04:40 – 05:00 **Joseph Lubin**: *Altering protease specificity with homologous loop substitution*
- 05:00 – 05:20 **Daniel Zaidman**: *Rational Design and Ternary Structure Prediction of PROTACs*

05:20 – 06:00 Keynote III: Session Chair: Moriah Longhurst

- **Eva-Maria Strauch**: *TBD*

06:00 – 06:10 Closing

- **Doug Renfrew & Julia Koehler Leman**: *Closing Remarks*
- Depart for dinner and events out on the town in NYC. Please make your choices here (https://docs.google.com/spreadsheets/d/17RktMG7XXnDo5sS-9j5GlN8OIszhO_N3m19rnLBgrKo/edit?usp=sharing)

Wednesday

Hotel check-out at noon

Dinner options

Dinner will be catered and covered by the conference. Just in case you need a bite close-by, here are some options. PLEASE KEEP IN MIND THAT ALCOHOL WILL NOT BE REIMBURSED!

- Sushi - Ootoya Chelsea, KazuNori
- Poke (ambiance is typically less inviting to stay longer) - PokeSpot or Pokeworks
- Pizza - Zero Otto Nove, PN Wood Fired Pizza
- Mediterranean - Hummus Kitchen (small), Byblos (pricey?)
- Indian - Mughlai, Pippali
- Thai - Thai Villa, ChaamLex, Spice, Ngam
- Burgers / American / BBQ - Ichabods, Cannibal Liquor House, Hardings
- Ramen / Noodles - Tsurutontan Udon, Ichiba, Kame Ramen
- Jewish deli - 2nd Ave Deli, Friedman's, Sarge's Delicatessen, Eisenberg
- Korean - Barn Joo (pricey), Five Senses, Her Name is Han, Soju Haus
- Asian/Fusion - Republic, Izakaya NoMad
- Mexican - Flats Fix Taqueria, Casa Neta, Oxido, Taco place in Chelsea market
- Seafood - Burger & Lobster, L & W Oyster Co., The Boil
- American/Tapas - The Cellar, The Smith

Full Group Discussion Topics

- What is Rosetta?
    - What's the limits of the Rosetta package? What counts as developing Rosetta proper versus developing a non-Rosetta thing which *uses* (Py)Rosetta?
    - If you make scripts (pre- & post-processing, XML, PyRosetta, etc.) when should they be officially part of Rosetta, and when should they be "extra" (external repos, supporting info, tarballs on lab webpages, etc.)?

- What infrastructure changes do we need to support the above? (new repos, testing hooks, distribution changes, etc.)
- How can we promote the cultural changes needed to support and maintain the above?
- Mac CPU time is expensive: should we stop running Mac integration/score tests and instead run a few more of them on different GCC on Linux?
- Right now integration test breakage in one of the thing that's trigger red-cross mark on PR which almost always there. Should we stop using integration tests results when calculating pass/fail for PR testing?
- GitHub labels: right now all GH labels triggers only sub-set of tests from default test set. Is it optimal for your workflow? If not, what labels / test-sets you would like to see?
- Our devel meetings now became less of devel meeting add more of RC: pre-RosettaCon at summer RC, - do we still need it?

TBD

Breakout session other topics

Hackathon

- Make an Exemplar Class
- Fix up {Rosetta,FoldIt,Rosetta@Home} Wikipedia pages
- Add/improve PyRosetta Notebooks (https://github.com/RosettaCommons/PyRosetta.notebooks) (Kathy Le, Jeff Gray)
- Fix permabroken and intermittently broken tests on test server (idea from Steven but TBH I will probably be running tutorials during this time frame not leading a hackathon)
  - Fix permabroken tests where possible (hackathon)
  - Brainstorm on the occasionally-broken ones (like PPI) to think up ways to trap or speedbump the trajectory issues
- your ideas here with names

Offer a Demo

- your name here

Science

- TBD

notes and summaries

WRC2020 summary Steven Lewis

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