CADD GRC 202X
Working together for a better tomorrow

John D. Chodera
Associate Member, Computational and Systems Biology Program
Sloan Kettering Institute, Memorial Sloan Kettering Cancer Center
http://www.choderalab.org


DISCLOSURES:
- Scientific Advisory Board, OpenEye Scientific
  All funding: http://choderalab.org/funding
My aim is to be a faithful steward of the CADD GRC and its inclusive, welcoming community.
BETTER INTEGRATING THE ACADEMY

Pair academic + industry talks
Supplement with key background material
Engage academics to focus on challenges that will have real impact
Short talks from talented young researchers
Preparing trainees for the transition into industry
- pair academic trainees with volunteer industry mentors
WE'RE ALL IN THE SAME BOAT
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THE LONELY ISLAND
I'M ON A BOAT
FEATURING T-PAIN

NO
A RISING TIDE LIFTS ALL BOATS
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How can we make the most of our time together as a community to make things better for everyone?
CEMENTING THE FUNDAMENTALS
Talks that empower our community to collaborate without friction, build on each other's work, and quickly identify significant improvements

Best practices for our craft
Recommended publication policies
Standards for interoperability
Community benchmark sets
Useful tools and frameworks
NEW TECHNOLOGIES

Talks that dive deeply into exciting new methods and technologies to get us thinking about how they will fit into the drug discovery and development paradigm

Automated chemistry and synthesis planning
Autonomous molecular design / self-driving labs
New structural methods: CryoEM and beyond
Integrative modeling of biochemical, structural, and biophysical data to support informed decisions
Machine learning isn't going away. But there is a lot of room between linear regression and irrational exuberance.

Deep dives on the fundamentals of ML relevant to chemistry and drug discovery

Machine learning is the new duct tape

How do we evaluate ML models?

How do we make models that are predictive?
LEARNING FROM FAILURES

Only by learning from failures can we transition from a research field into an engineering field. How can we change our culture to extract value from failure?
CHALLENGES LACKING SOLUTIONS

Talks that highlight unmet needs in our discipline, educate us about unfamiliar important problems, and inspire innovation in new areas.
We're no longer living in the 19th century

https://colinpurrington.com/tips/poster-session/
ALSO: PLACEMATS