CMACS

Computational **M**odeling and **A**nalysis for **C**omplex **S**ystems

2012 Workshop on Signaling Pathways and Pancreatic Cancer

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April 19, 2012

Acknowledgments

- James Faeder
- Leonard Harris and Justin Hogg
- Bud Mishra
- Ilya Korsunsky
- Haijun Gong
- Ilya Nemenman
- Terri Grosso, Kai Zhao, Aron Wolinetz

Innovations

- **Broadcast and recording of workshop**
  - Videos will be available by June
  - Audio is tough for interactive style
- **Looser definition of group work**
  - Pushed by students
  - Effective
- **Continued engagement in active research**

Outline

- **Objectives**

- **Approach**

- Students

- Outcomes

Objectives

1. Exposing students to research
2. Engaging students in research
3. Acquainting students with collaborative work
4. Promoting STEM fields
5. Engaging under-represented groups

Objective 5 – Engaging Under-represented Groups

Hispanic	5
African-American	1
Women	7

Objective 4 – Promote STEM

- Two students working with Expedition groups (Mishra, Griffeth)

- Faeder will hire at least one student as a summer intern

- One more student is interested but must be paid

- Other students are looking for STEM internships

Objective 4 – Promote STEM

"The workshop helped me to understand":

how to analyze and use models of biological processes	4.6 (5)
biological processes	4.4 (5)
how to construct and use models of biological processes	4.4 (5)
how to simulate biological processes	4.7 (5)
how to formulate and examine scientific hypotheses	4.1 (4)
how scientific research works	4.6 (5)
I feel more confident of my ability to do scientific or technical work as a result of attending the workshop	4.7 (5)
The workshop was a worthwhile way of spending my time	4.8 (5)
I would be interesting in attending another such workshop	4.4 (5)
The workshop made me more interested in continuing my schooling in a scientific, technical, engineering, or mathematical field	4.5 (5)

Approach – Objective 3 (Collaboration)

- **Approach:**
  - Organize into teams for projects
  - Model Sort Exercise – what are the most important properties of a model?

- **Outcomes: Teamwork and Evaluations**

Objective 3 – Collaboration

- From the evaluation, "Best thing about the workshop"
  - "Being able to work with smart people from other majors on a project that spanned topics out of the range of my major."
  - "The open-learning environment and sharing knowledge with so many really, really smart and great people."
  - "I loved working with people from different backgrounds and interest. I really appreciated my colleagues helping me better understand the biology behind our experiments."
 - "Working with highly motivated students from different backgrounds was very inspiring and eye-opening."

Approach – Objectives 1 and 2 (Research)

- **Approach:**
  - Keynote talks from active researchers
  - Student Projects, with potential for contributing to active research
- **Outcomes:** Student Presentations, publication

Research Problem

- Coarse-graining of simulations

- Approach: represent an entire chain of chemical reactions with a single distribution function

- Student problem: develop cdf's through stochastic simulations rather than analytically

Project: EGFR Pathway

Group: : Melanie Balmick
Hery Ratsimihah
Rachel Spratt

EGF Probability Distribution
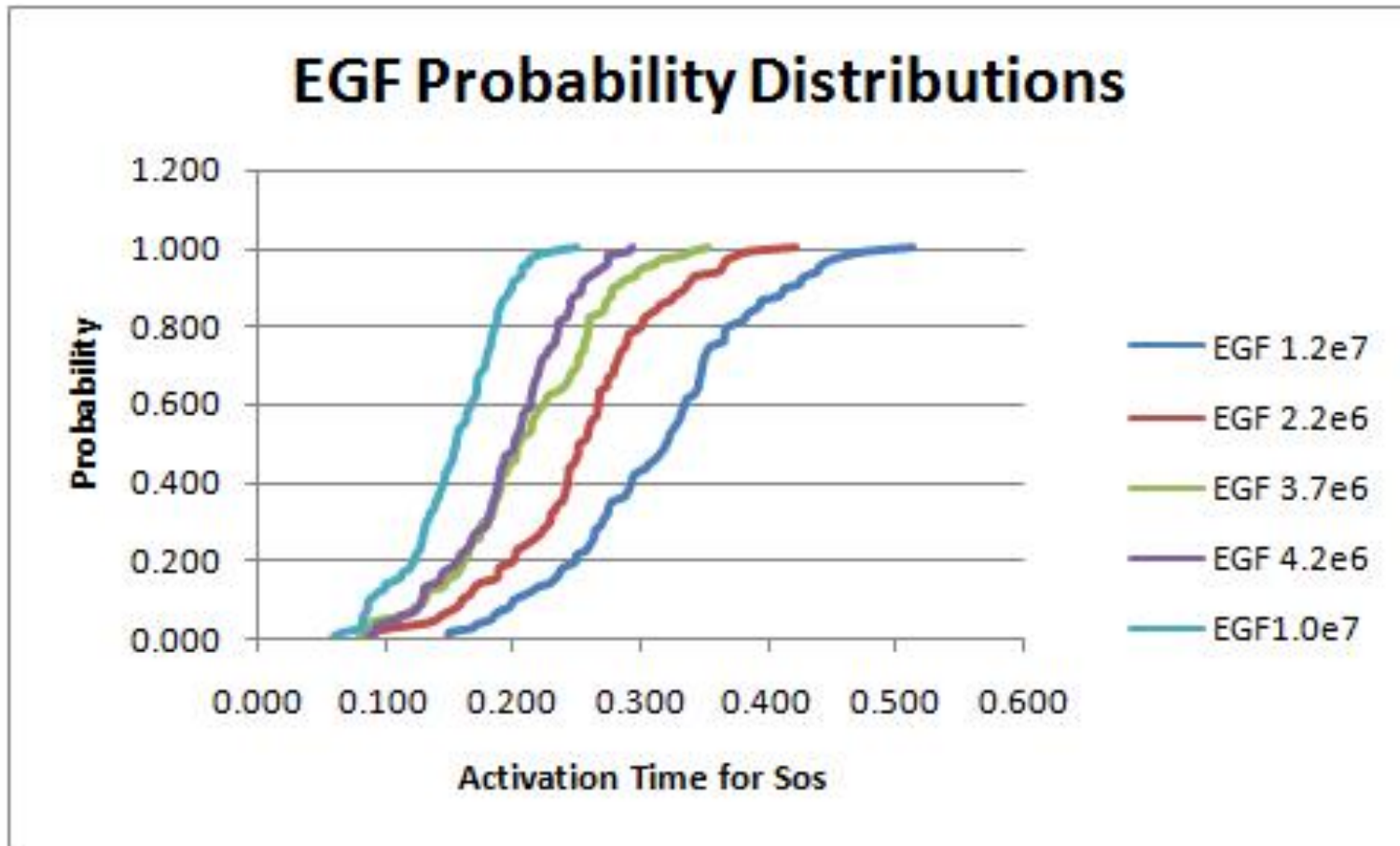
The translation of CDF curves, due to the change in concentration, illustrates how concentration effects Sos activation time.
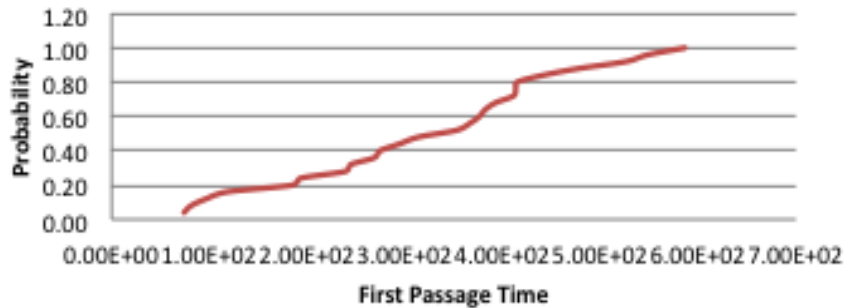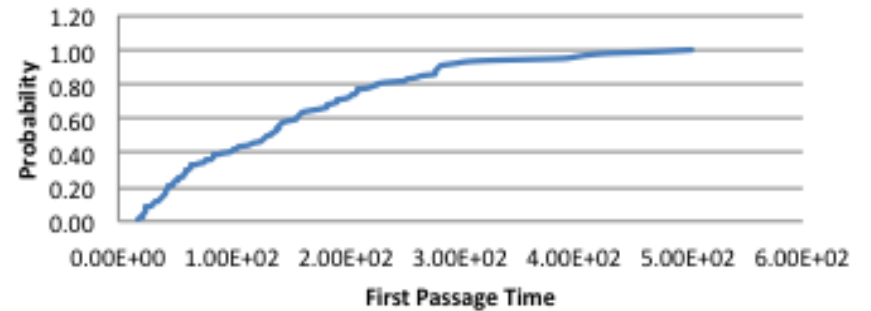
13
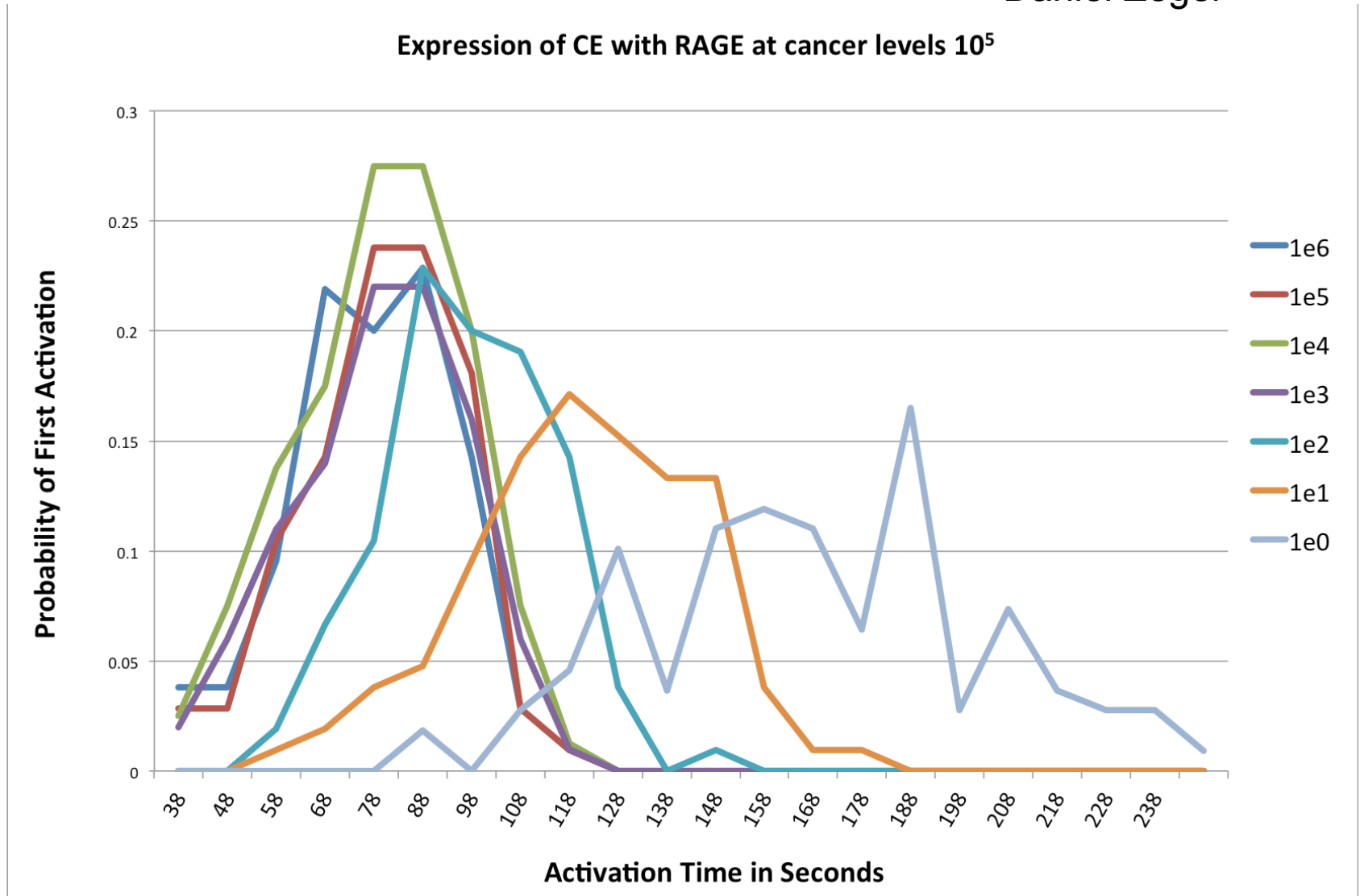
Project: FcεRI Pathway

Group: Anna Feitzinger
Axel Nunez
Farah Abbasi

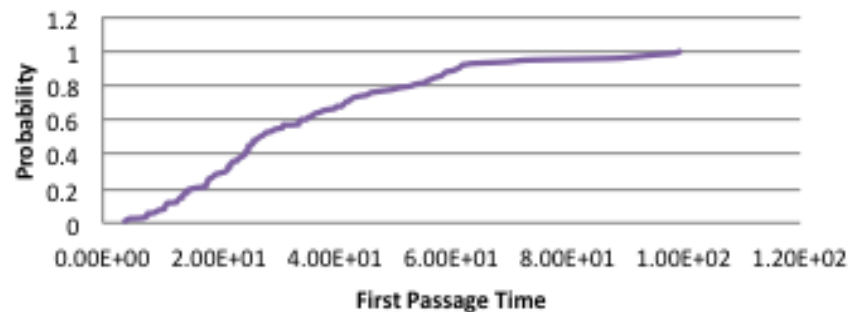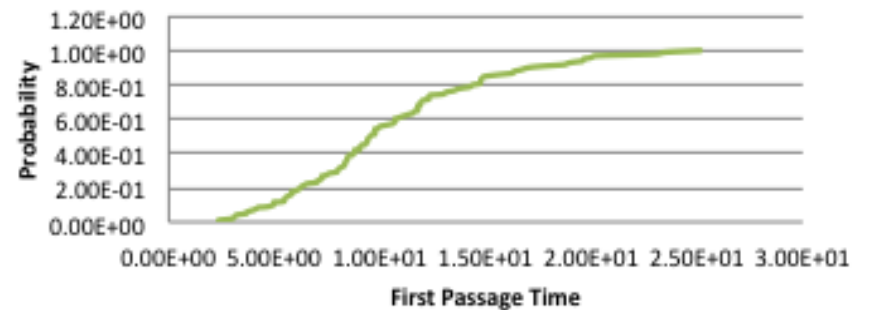CDF: First Passage Time for the Phosphorylation of Syk with an [IgE] 6 (100 runs)

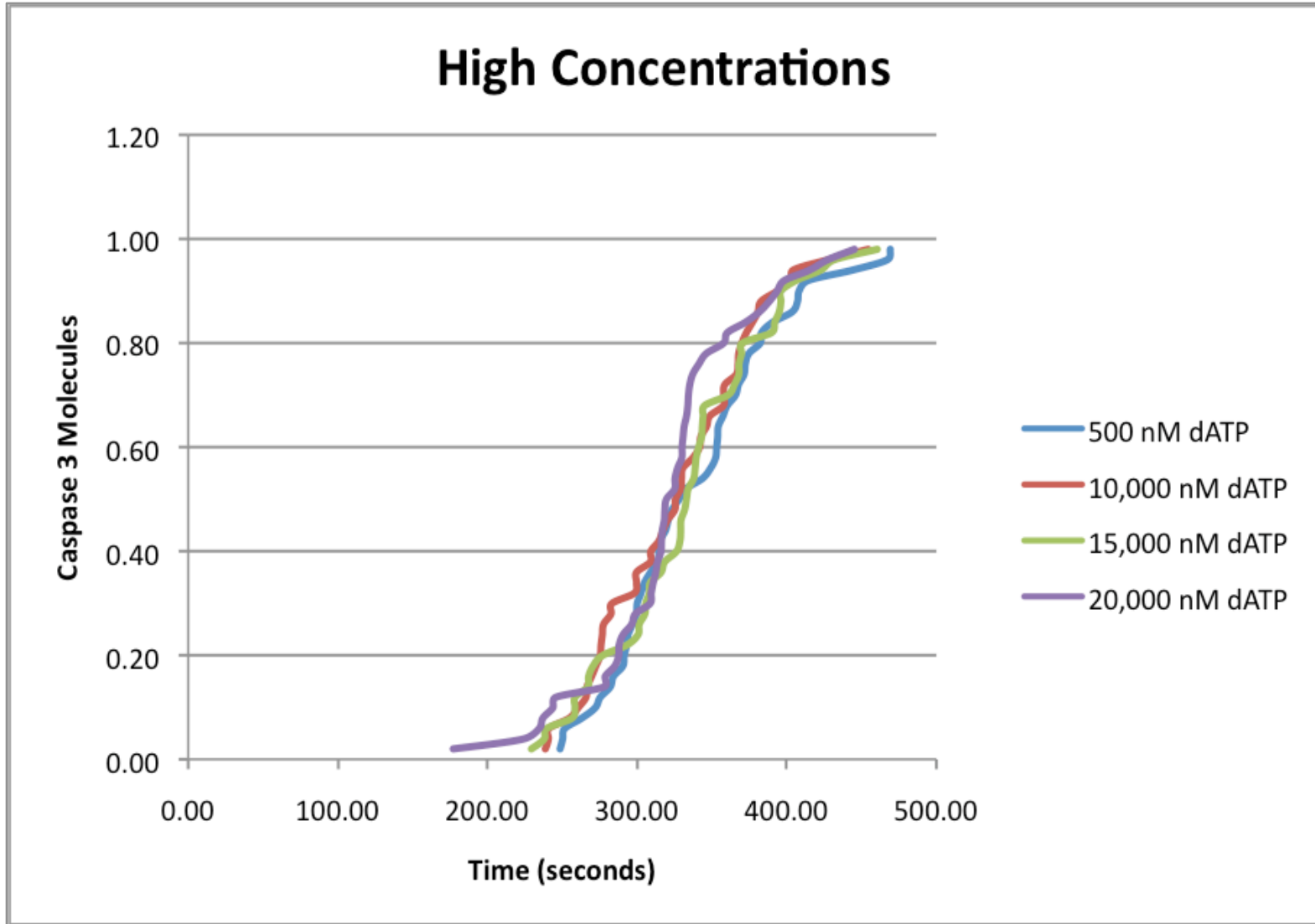CDF: First Passage Time for the Phosphorylation of Syk with an [IgE] 60 (100 runs)

CDF: First Passage Time for the Phosphorylation of Syk with an [IgE] 600 (100 runs)

CDF: First Passage Time for the Phosphorylation of Syk with an [IgE] 6000 (100 runs)
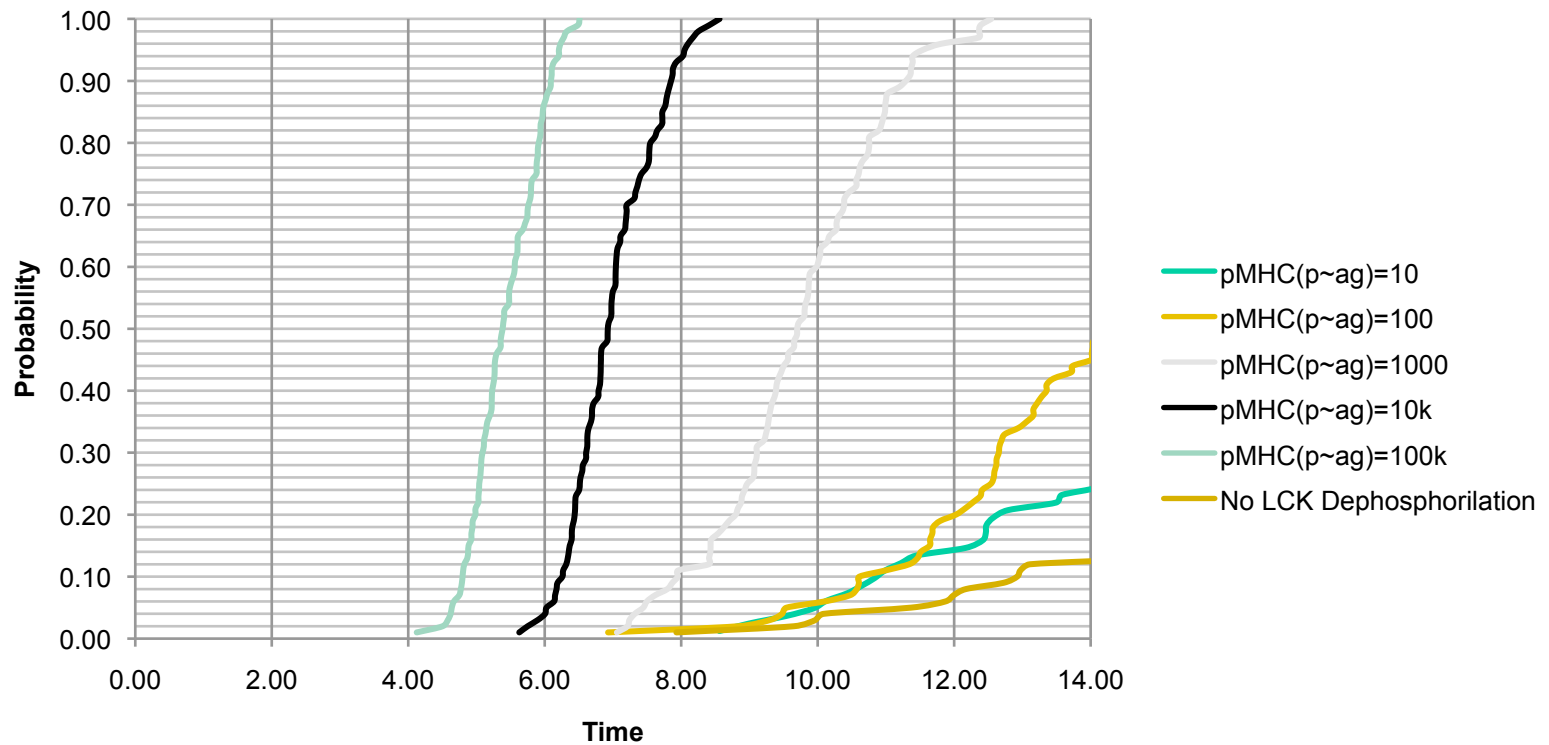
Project: Apoptosis pathways

Group: Marieta Garib
Aisha Green
Linda Miranda

High Concentrations

Caspase 3 Molecules vs Time (seconds)

- 500 nM dATP
- 10,000 nM dATP
- 15,000 nM dATP
- 20,000 nM dATP

Results

Cumulative Distribution

Legend:
- pMHC(p~ag)=10
- pMHC(p~ag)=100
- pMHC(p~ag)=1000
- pMHC(p~ag)=10k
- pMHC(p~ag)=100k
- No LCK Dephosphorilation

Video

- Adobe Connect
- Challenge: Need to record without affecting workshop quality
- Audio problems
  - Need more mics
  - Remote participant problems – Skype better!
- For movies: Adobe Connect requires real-time download!!

Summary

- **Another success**
  - Great students
  - Great help from grad students and colleagues – Terri Grosso, Kai Zhao, Aron Wolinetz, Jim Faeder, Bud Mishra, Ilya Nemenman, and all of Jim's group, especially Leonard Harris and Justin Hogg
- **See facebook "NSF CMACS"**