

# 3<sup>rd</sup> Annual Interdisciplinary Quantitative Biology **BOOT CAMP**

## **DRUG DISCOVERY AND DEVELOPMENT**

## PROGRAM

### **January 4–15, 2016**

**Center for Integrative Proteomics Research**

Rutgers University • Busch Campus

174 Frelinghuysen Rd

Piscataway, NJ 08854-8076

[iqb.rutgers.edu/bootcamp](http://iqb.rutgers.edu/bootcamp)



Institute for Quantitative  
Biomedicine at Rutgers

Graduate Program in  
Quantitative Biomedicine



Center for Integrative  
**PROTEOMICS**  
Research

**RUTGERS**  
THE STATE UNIVERSITY  
OF NEW JERSEY

## Interdisciplinary Quantitative Biology Boot Camp Drug Discovery and Development

The Center for Integrative Proteomics Research, home to the Institute for Quantitative Biomedicine, and the Graduate Program in Computational Biology and Molecular Biophysics (soon to be renamed the Graduate Program in Quantitative Biomedicine), are delighted to be hosting the Third Annual Rutgers Interdisciplinary Quantitative Biology Boot Camp in Drug Discovery and Design. Boot Camp is designed to augment education for quantitative and biological scientists. Our overarching goal is to introduce students of all ages to the value of integrating biology and medicine with mathematics, physics, chemistry, computer science, statistics and biostatistics, and engineering.

The immersive two-week Boot Camp will provide broad introductory exposure to the language, culture, and experimental/theoretical underpinnings of molecular biology, macromolecular biochemistry/biophysics, structural biology, computational biology, systems biology, and bioinformatics.

Instruction will take the form of lectures on the A-to-Z of drug discovery and development as well as a broad range of collaborative hands-on workshops for simulating the qualities of the small molecules under study as well as their interactions with target molecules and the more complex hosts and populations within which they operate. There will also be career development activities, tours of some of Rutgers' state-of-the-art facilities for interrogating biological phenomena, student-driven topics-of-the-day, fun activities for relaxing, and two end-of-week networking opportunities.

The final afternoon of the Boot Camp will be devoted to a student-led simulation of a so-called briefing package and an Oncologic Drugs Advisory Committee (ODAC) meeting, key prerequisites for getting FDA approval. This event will involve a cooperative synthesis of the material covered in the two-week program.

The Boot Camp would not have been possible without tireless efforts of more than sixty contributors from across Rutgers and from our partners at Merck, Bristol-Meyers Squibb, Colgate-Palmolive, Novartis, the Novartis Institutes for Biomedical Research, the Cambridge Crystallographic Data Centre, Fox Rothchild LLP, and Landing Expert Career Coaching.

Special thanks go out to Luz Fajardo, Kenneth Dalenberg, Bernie Cariaga, Jonathan Hackett, and Don Corrette of the Center for Integrative Proteomics Research as well as students Krupa Shah, Maria Qadri, Kathryn Drzewiecki, Chris Wakim, Domonick Panzera, Grant Bilker, Sophia Tan, and Ryan Woltz.

Note:

All sessions will be held in  
**PROTEOMICS, ROOM 120**  
 unless designated otherwise



Laptop computers are required for sessions designated with this icon

Monday, January 4<sup>th</sup>, 2016

MORNING

9:00 AM	<b>Welcome and Orientation</b> Gail Ferstandig Arnold, IQB
9:10 AM	<b>Nexus of Academe and Drug Discovery and Development</b> Christopher Molloy, ORED
9:30 AM	<b>What is Cancer?</b> Shridar Ganesan, CINJ
10:30 AM	<i>Coffee/Tea Served</i>
10:50 AM	<b>What is a Drug? What is Discovery? What is Development?</b> David Kimball, ORED
11:40 AM	<b>What is Precision Medicine?</b> Robert DiPaola, CINJ

AFTERNOON

12:30 PM	<i>Lunch Served – Proteomics First Floor Lobby</i>
1:30 PM	<b>Career Byte: Branching Out: Meeting Colleagues</b> Maria Qadri, BME
2:30 PM	<b>NewCo Organization</b> Stephen K. Burley/Gail Ferstandig Arnold, IQB <ul style="list-style-type: none"> <li>• Review of Boot Camp program and goals</li> <li>• Organizing participants into NewCo</li> </ul>
3:30 PM	<b>Target Exploration Workshop</b> Michael Fitzgerald, Colgate-Palmolive <ul style="list-style-type: none"> <li>• Is the EGF/EGFR signaling pathway a sensible target for treating cancer?</li> </ul> Coffee/Tea available throughout afternoon
4:30 PM	Dinner Served - <i>Proteomics First Floor Lobby</i> <b>Trivia for Scientists</b>

Tuesday, January 5<sup>th</sup>, 2016

MORNING

9:00 AM	<b>NewCo Report</b> Participants
9:15 AM	<b>Signaling Pathways Central to Cell Growth and EGF/EGFR</b> Steven Zheng, CINJ
10:00 AM	<b>Initiating a Protein Kinase Drug Discovery Program I</b> Peter Young, Biotech Executive and Consultant
10:45 AM	Coffee/Tea Served
11:05 AM	<b>Initiating a Protein Kinase Drug Discovery Program II</b> Peter Young, Biotech Executive and Consultant



11:50 AM *Lunch (independent)*

AFTERNOON

12:40 PM	 <b>Career Byte: Mapping Out Opportunities Ahead</b> Toi Tyson, Rutgers Career Office; Michael Fitzgerald/Hallie Strotman/Camille Zenobia, Colgate-Palmolive
1:10 PM	<b>NewCo Meeting</b> Stephen K. Burley/Gail Ferstandig Arnold, IQB
1:40 PM	 <b>EGFR Molecular Visualization Workshop</b> Shuchismita Dutta/Luigi DiCostanzo, RCSB PDB
3:10 PM	Coffee/Tea Served
3:30 PM	 <b>Amber Workshop: Simulating EGFR Breathing and Potential for Drug Binding, Part I</b> David Case/Darrin York/Jason Swails/Hai Nguyen, CCB/Proteomics



Wednesday, January 6<sup>th</sup>, 2016

MORNING

9:00 AM	<b>NewCo Report</b> Participants
9:05 AM	<b>What is Medicinal Chemistry?</b> David Kimball, ORED
9:50 AM	<b>Kinase Inhibitor Lead Discovery</b> John Tokarski, BMS
10:35 AM	Coffee/Tea Served
10:55 AM	 <b>Cambridge Crystallographic Data Centre</b> Amy Sarjeant, CCDC
11:25 AM	 <b>Medicinal Chemistry Workshop Orientation</b> John Westbrook, RCSB PDB

12:10 PM *Lunch (independent)*

AFTERNOON

1:00 PM	 <b>Career Byte:</b> <ul style="list-style-type: none"> <li>• <b>Organization: A Way to Brand Yourself as Someone who is Responsible and Balanced</b> Emily Arnold, RU School of Social Work</li> <li>• <b>Rutgers iJOBS</b> Janet Alder, NCB, GASA, RWJMS</li> </ul>
1:30 PM	<b>NewCo Meeting</b> Stephen K. Burley/Gail Ferstandig Arnold, IQB
2:00 PM	 <b>In silico Medicinal Chemistry Workshop</b> David Augeri, Translational Sciences; Lawrence Williams, CCB; Shashidhar Rao, Proteomics; John Westbrook, RCSB PDB Coffee/Tea available throughout afternoon

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4:00 PM Dinner Served - *Proteomics Lobby*  
**Boot Camp Machinations**

# WEEK 1 • January 4 - 8, 2016

## Thursday, January 7<sup>th</sup>, 2016

MORNING

9:00 AM	<b>NewCo Report</b> Participants
9:05 AM	<b>ADME</b> (Absorption/Distribution/Metabolism/Excretion) Imad Hanna, Novartis
10:05 AM	Coffee/Tea Served
10:35 AM	<b>Small Molecule Pharmacokinetics (PK)</b> Ry Forseth, Novartis
11:35 AM	<b>Small Molecule Pharmacodynamics (PD)</b> Christina Won, Novartis

12:15 PM *Lunch (independent)*

AFTERNOON

1:15 PM	<b>Career Byte: Securing an Industrial Position: A Hiring Manager's Perspective</b> Joseph Duffy, Merck
1:45 PM	 <b>PK/PD Modeling Workshop</b> Ry Forseth/Christina Won, Novartis Coffee/Tea available throughout afternoon
3:30 PM	<b>NewCo Meeting</b> Stephen K. Burley/Gail Ferstandig Arnold, IQB


## Friday, January 8<sup>th</sup>, 2016

MORNING

9:00 AM	<b>NewCo Report</b> Participants
9:05 AM	<b>Ethics Considerations/Informed Consent/Institutional Review Boards</b> Eric Singer, CINJ
10:05 AM	Coffee/Tea Served
10:25 AM	<b>The Why, When, What of Toxicology Testing in Drug Discovery and Development</b> Sudheer Beedanagari, Bristol-Myers Squibb
11:25 AM	<b>Selecting the Oncology Drug Candidate</b> Louis Lombardo, Bristol-Meyers Squibb

12:25 PM *Lunch (independent)*

AFTERNOON

1:30 PM	<b>Career Byte:</b> • <b>Making a Winning CV</b> Mike Kiledjian, CBN • <b>GradFund</b> Teresa DelCorso Ellmann, GSNB
2:00 PM	<b>NewCo Meeting</b> Stephen K. Burley/Gail Ferstandig Arnold, IQB
2:30 PM	 <b>Tumor Genome Profiling Workshop</b> Chang Chan/Saurabh Laddha, CINJ Coffee/Tea available throughout afternoon

4:30 PM **Networking Event;** Dinner Served - *Proteomics Lobby*

# WEEK 2 • January 11 - 15, 2016

## Monday, January 11<sup>th</sup>, 2016

MORNING

- 9:00 AM **NewCo Report** Participants
- 9:15 AM **An Academia/Pharma Partnership that Led to Three Marketed Drugs for Treating HIV Infection** Eddy Arnold, CABM/CCB/Proteomics
- 10:10 AM Coffee/Tea Served
- 10:30 AM **Patenting the Drug Candidate**  
Vincent Smeraglia, ORC/Peter Butch, Esq., Fox Rothschild
- 11:30 AM **NewCo Meeting** Stephen K. Burley/Gail Ferstandig Arnold, IQB

12:00 PM *Lunch (independent)*

AFTERNOON

- 1:00 PM **Career Byte: Giving an Engaging Presentation or Pitch**  
Jerome Kukor, GSNB
- 1:30 PM  **Tumor Transcriptome Profiling Workshop**  
Chang Chan/Saurabh Laddha, CINJ
- 3:15 PM Coffee/Tea Served
- 3:35 PM  **Amber Workshop: Simulating EGFR Breathing and Potential for Drug Binding, Part II**  
David Case/Darrin York/Jason Swails/Hai Nguyen, CCB/Proteomics
- 4:30 PM PB & J and Popcorn - **Proteomics Lobby**; ODAC Movie/Think Tank Forum


## Tuesday, January 12<sup>th</sup>, 2016

MORNING

- 9:00 AM **NewCo Report** Participants
- 9:05 AM **Preparing the Investigational New Drug Application (IND)**  
Stephen K. Burley, Proteomics/IQB
- 9:30 AM **Design and Conduct of Phase 1/2 Clinical Trials** Julie Reynes, Novartis
- 10:30 AM Coffee/Tea Served
- 11:00 AM **Design and Conduct of Phase 3 Clinical Trials** Julie Reynes, Novartis
- 11:30 AM **Preparing the New Drug Application (NDA)**  
Stephen K. Burley, Proteomics/IQB

12:00 PM *Lunch (independent)*

AFTERNOON

- 1:00 PM **Career Byte: The Interview: You Are Onstage**  
Alex Freund, Landing Expert Career Coaching
- 2:00 PM Coffee/Tea Served
- 2:30 PM **NewCo Meeting** Stephen K. Burley/Gail Ferstandig Arnold, IQB
- 3:00 PM **Kinase Inhibitor Resistance** Steven Zheng, CINJ
- 4:00 PM  **Tumor Proteome Profiling Workshop** Justin Drake, CINJ

MORNING

- 9:00 AM **NewCo Report** Participants
- 9:15 AM **Statistical Analysis Workshop: Analysis of Tumor Profiling Data**  
Steve Buyske, HGINJ
- 10:30 AM Assemble in **front of Proteomics** for walk to tours:
- **Keck Center for Collaborative Neuroscience**  
Patricia Morton, Spinal Cord Injury Project  
(offered at 10:45 AM only)
  - **Applications of Quantitative Biology to Environmental Health**  
Panos Georgopoulos, EOHSI
  - **RD12: A Look behind the Scenes at Advanced Computing**  
Moustafa AbdelBaky, ECE

10:45 AM  
11:45 AM

**Tour 1**  
**Tour 2**

**OPTIONS**

Tour 1                      Tour 2

1. Keck Center → EOHSI
2. Keck Center → RD12
3. EOHSI → RD12
4. RD12 → EOHSI

AFTERNOON

1:00 PM *Lunch (independent)*

2:00 PM **Career Byte: Using Social Media to Your Advantage**  
Ina Nikolaeva, MMG

2:30 PM **NewCo Meeting** Stephen K. Burley/Gail Ferstandig Arnold, IQB

3:30 PM **Preparation for Briefing Package/Oncologic Drugs Advisory Committee Simulation**

Coffee/Tea available throughout afternoon

5:00 PM **Downtown Meeting**  
Meet in Proteomics Lobby

Thursday, January 14<sup>th</sup>, 2016

MORNING

9:00 AM **NewCo Report** Participants  
 9:15 AM Assemble in **front of Proteomics** for walk to tours:  
 • **RUCDR Infinite Biologics: A Full Service Biorepository for the 21st Century** Michael Sheldon, RUCDR;  
 • **Bioimaging** Carol Gardner/Jessica Cervelli, Pharmacy  
 9:30 AM **Tour 1**  
 10:30 AM **Tour 2**

**OPTIONS**

Tour 1                      Tour 2

1. RUCDR      -> Bioimaging
2. Bioimaging -> RUCDR

AFTERNOON

11:40 AM **ORED Internship Program** Tatiana Litvin-Vechnyak, OTC

12:40 PM *Lunch (independent)*

1:30 PM  **Career Byte: Finding Jobs and Collaborators Using LinkedIn**  
 Itzamarie Chevere-Torres, Genetics

2:00 PM **Preparation for Briefing Package/Oncologic Drugs Advisory Committee Simulation**  
 Coffee/Tea available throughout afternoon

Friday, January 15<sup>th</sup>, 2016

MORNING

9:00 AM **Finalization of Presentation for the Briefing Package/Oncologic Drugs Advisory Committee Simulation**  
 Coffee/Tea available throughout morning

12:00 PM *Lunch Served - Eat in 9 career groupings, Proteomics Lobby*

1:00 PM **Main Event: Briefing Package/Oncologic Drugs Advisory Committee Simulation**

2:30 PM Coffee/Tea Served

AFTERNOON

3:00 PM **Networking/Career Fair/"Speed Dating" Style Meet and Greets**  
 Dinner Served with Special Dessert - *Proteomics Lobby*



## **Moustafa AbdelBaky, Ph.D. Candidate**

Electrical and Computer Engineering  
Rutgers University

## **Janet Alder, Ph.D.**

Associate Professor, Neuroscience and Cell Biology  
Assistant Dean, Graduate Academic and Student Affairs  
Rutgers Robert Wood Johnson Medical School

## **Eddy Arnold, Ph.D.**

Board of Governors Professor, Chemistry and Chemical Biology  
Member, Center for Advanced Biotechnology and Medicine  
Member, Center for Integrative Proteomics Research  
Member, Rutgers Cancer Institute of New Jersey  
Rutgers University

## **Emily Arnold, B.S.**

Masters Student of Social Work  
Rutgers University

## **Gail Ferstandig Arnold, Ph.D.**

Associate Director, Institute for Quantitative Biomedicine  
Associate Director of Graduate Studies, Computational Biology and Molecular Biophysics/  
Quantitative Biomedicine  
Rutgers University

## **David J. Augeri, Ph.D**

Director of Molecular Design and Synthesis  
Research Professor I  
Ernest Mario School of Pharmacy  
Rutgers University

## **Sudheer Beedanagari Ph.D.**

Research Investigator II, Genetic Toxicology  
Drug Safety Evaluation  
Bristol-Myers Squibb

## **Jim Bennett, B.S.**

Program Coordinator, Spinal Cord Injury Project  
W.M. Keck Center for Collaborative Neuroscience  
Rutgers University

## **Grant Bilker**

Undergraduate Student  
Rutgers University

## **Andrew Brooks, Ph.D.**

Associate Research Professor, Genetics  
Chief Operating Officer, Rutgers University Cell and DNA Repository  
Director, Bionomics Research and Technology Center  
Rutgers University

## **Stephen K. Burley, M.D., D. Phil.**

Director, Center for Integrative Proteomics Research  
Founding Director, Institute for Quantitative Biomedicine  
Director, Research Collaboratory for Structural Bioinformatics Protein Data Bank  
Distinguished Professor, Chemistry and Chemical Biology  
Member, Rutgers Cancer Institute of New Jersey  
Rutgers University

## **Peter Butch, J.D.**

Partner at Fox Rothschild LLP

## **Steve Buyske, Ph.D.**

Associate Research Professor, Statistics and Biostatistics  
Rutgers University

## **Bernadette Cariaga, C.P.A.**

Business Manager, Center for Integrative Proteomics Research  
Rutgers University

## **David A. Case, Ph.D.**

Distinguished Professor, Chemistry and Chemical Biology  
Member, Proteomics  
Rutgers University

## **Jessica Cervelli**

Laboratory Technician  
Pharmacology and Toxicology Department  
Ernest Mario School of Pharmacy  
Rutgers University

## **Chang S. Chan, Ph.D.**

Assistant Professor of Medicine  
Full Member, Rutgers Cancer Institute of New Jersey  
Rutgers Robert Wood Johnson Medical School

## **Itzamarie Chevere-Torres, Ph.D.**

Postdoctoral Associate, Genetics Department  
Rutgers University

## **Don Corrette**

Building Manager, Center for Integrative Proteomics Research  
Rutgers University

## **Kenneth Dalenberg**

Unit Computing Specialist, Center for Integrative Proteomics Research  
Rutgers University

## **Luigi DiCostanzo, Ph.D.**

Research Associate, Chemistry and Chemical Biology  
Biocurator, Research Collaboratory for Structural Bioinformatics Protein Data Bank  
Rutgers University

**Teresa Delcorso Ellmann**

Assistant Dean, Graduate School-New Brunswick  
Director, GradFund  
Rutgers University

**Robert S. DiPaola, M.D.**

Director, Rutgers Cancer Institute of New Jersey  
Vice Chancellor for Cancer Programs, Rutgers Biomedical and Health Sciences  
Professor of Medicine  
Rutgers Robert Wood Johnson Medical School

**Justin M. Drake, Ph.D.**

Assistant Professor of Medicine  
Full Member, Rutgers Cancer Institute of New Jersey  
Rutgers Robert Wood Johnson Medical School

**Kathryn Drzewiecki, Ph.D. Candidate**

Biomedical Engineering and Quantitative Biomedicine  
Philanthropic Educational Organization Scholar  
Rutgers University

**Joseph L. Duffy, Ph.D.**

Executive Director of Discovery Chemistry  
Merck Research Labs, Rahway, NJ

**Shuchismita Dutta, Ph.D.**

Assistant Research Professor, Chemistry and Chemical Biology  
Senior Educational Coordinator, Research Collaboratory for Structural Bioinformatics Protein Data Bank  
Rutgers University

**Luz A. Fajardo, B.S.**

Administrative Assistant, Center for Integrative Proteomics Research  
Rutgers University

**Michael Fitzgerald, B.S.**

Research Scientist  
Colgate-Palmolive

**Ry Forseth, Ph.D.**

Investigator II  
Novartis Pharmaceuticals

**Alex Freund, B.S.**

Founder and Career Coach, Landing Expert Career Coaching

**Shridar Ganesan, M.D., Ph.D.**

Director of Functional Genomics Shared Resource  
Associate Director, Translational Science  
Section Chief, Cancer Biology at Rutgers Cancer Institute of New Jersey  
Full Member, Rutgers Cancer Institute of New Jersey  
Omar Boraia Chair in Genomic Science, Associate Professor of Medicine and Pharmacology  
Rutgers Robert Wood Johnson Medical School

## **Carol Gardner, Ph.D.**

Associate Research Professor, Pharmacology and Toxicology  
Ernest Mario School of Pharmacy  
Rutgers University

## **Panos G. Georgopoulos, Ph.D.**

Director, Computational Chemodynamics Laboratory  
Director, Ozone Research Center and the Informatics and Computational Toxicology Core  
Professor, Environmental and Occupational Health at Rutgers Biomedical and Health Sciences  
Environmental and Occupational Health Sciences Institute  
Rutgers University

## **Imad Hanna, Ph.D.**

Director, Drug Metabolism and Pharmacokinetics  
Novartis Institutes for BioMedical Research

## **Megerditch (Mike) Kiledjian, Ph.D.**

Distinguished Professor and Chair, Cell Biology and Neuroscience  
Rutgers University

## **S. David Kimball, Ph.D.**

Associate Vice President, Translational Research, Office of Research Commercialization  
Research Professor, Medicinal Chemistry  
Ernest Mario School of Pharmacy  
Member, Rutgers Cancer Institute of New Jersey  
Rutgers University

## **Jerome Kukor, Ph.D.**

Dean of the Graduate School - New Brunswick  
Professor, Environmental Science  
Rutgers University

## **Saurabh Laddha, M.S.**

Graduate Student, Quantitative Biomedicine  
Rutgers Cancer Institute of New Jersey  
Rutgers University

## **Debra Laskin, Ph.D.**

Distinguished Professor and Roy A. Bowers Endowed Chair, Pharmacology and Toxicology  
Ernest Mario School of Pharmacy  
Rutgers University

## **Catherine Lawson, Ph.D.**

Associate Research Professor, Chemistry and Chemical Biology  
Rutgers University

## **Tatiana Litvin-Vechnyak, Ph.D.**

Associate Director, Office of Research Commercialization  
Director, Biomedical and Life Sciences Licensing  
Rutgers University

**Louis J. Lombardo, Ph.D.**

Group Director, Immunology Chemistry  
Bristol-Meyers Squibb

**John McCauley, Ph.D.**

Director, Medicinal Chemistry  
Merck Research Labs, West Point, PA

**Christopher J. Molloy, Ph.D., R.Ph.**

Senior Vice President, Office of Research and Economic Development  
Distinguished Professor, Pharmacology and Toxicology  
Rutgers University

**Patricia Morton, Ph.D.**

Director, Planning and Development  
The Spinal Cord Injury Project  
W. M. Keck Center for Collaborative Neuroscience  
Rutgers University

**Harry Namkoong, B.S.**

System Administrator, Center for Integrative Proteomics Research  
Rutgers University

**Hai Nguyen, Ph.D.**

Postdoctoral Research Fellow, Chemistry and Chemical Biology  
Rutgers University

**Jude Ndubuisi Okonne, Videographer**

Undergraduate Student  
Rutgers University

**Ina Nikolaeva, Ph.D. Candidate**

Cell Biology and Neuroscience  
Rutgers University

**Dominick Panzera, B.S.**

Rutgers University

**Maria Qadri, M.S., Ph.D. Candidate**

Biomedical Engineering and Quantitative Biomedicine  
Graduate Student Fellow, Rutgers Academy for the Scholarship of Teaching and Learning  
Rutgers University

**Shashidhar Rao, Ph.D.**

Scientist, Chemistry and Chemical Biology  
Rutgers University

**Julie Reynes, M.B.A.**

Global Trial Leader  
Novartis Pharmaceuticals

**Melissa Romanus, Ph.D. Candidate**

Electrical and Computing Engineering and Quantitative Biomedicine  
XSEDE Student Scholar  
Rutgers University

**Amy Sarjeant, Ph.D.**

Outreach and Education Manager  
The Cambridge Crystallographic Data Centre

**Eric A. Singer, M.D., M.A.**

Full Member, Rutgers Cancer Institute of New Jersey  
Rutgers Robert Wood Johnson Medical School

**Michael Sheldon, Ph.D.**

Director, RUCDR Infinite Biologics Stem Cell Laboratory  
Associate Research Professor, Department of Genetics  
Rutgers University

**Vincent Smeraglia, J.D.**

Executive Director of Strategic Alliances  
Office of Research Commercialization  
Rutgers University

**Jason Swails, Ph.D.**

Postdoctoral Research Fellow, Chemistry and Chemical Biology  
Rutgers University

**Sophia Tan, B.S.**

Rutgers University

**Jay Tischfield, Ph.D.**

Director, RUCDR Infinite Biologics  
Executive Director, Human Genetics Institute of New Jersey  
Distinguished Professor, Genetics  
Rutgers University

**John S. Tokarski, Ph.D.**

Senior Research Investigator, Molecular Discovery Technologies  
Bristol-Myers Squibb

**Toi Tyson, M.A.**

Assistant Director for Alumni Engagement and Graduate Student Programs  
Career Development & Experiential Education  
Rutgers University

**Maria Voigt, M.A.**

Outreach Coordinator, Research Collaboratory for Structural Bioinformatics Protein Data Bank  
Rutgers University

**Chris Wakim**

Undergraduate  
ARESTY Fellow  
Rutgers University

**Christina Won, Pharm.D., Ph.D.**

Senior Scientist  
Oncology Clinical Pharmacology  
Novartis Pharmaceuticals

**John Westbrook, Ph.D.**

Research Professor, Chemistry and Chemical Biology  
Principal Scientific Application/Web Developer and Architect, Research Collaboratory for  
Structural Bioinformatics Protein Data Bank  
Rutgers University

**Lawrence Williams, Ph.D.**

Professor, Chemistry and Chemical Biology  
Rutgers University

**Ryan Woltz, Ph.D. Candidate**

Chemistry and Chemical Biology  
Rutgers University

**Darrin York, Ph.D.**

Professor, Chemistry and Chemical Biology  
Member, Center for Integrative Proteomics Research  
Rutgers University

**Peter R. Young, Ph.D.**

Biotech Executive and Consultant

**Steven Zheng, Ph.D.**

University Professor and Chief, Division of Cancer Pharmacology  
Co-Leader, Cancer Pharmacology Program  
Rutgers Cancer Institute of New Jersey  
Rutgers Robert Wood Johnson Medical School

# RUTGERS BUSCH CAMPUS MAP

- Center for Integrative Proteomics Research (Proteomics)
- Parking with valid Faculty/Staff Permit
- Parking with valid Student Permit
- Bus Stop

