RUTGERS

PYTHON SCRIPTING for Biochemistry & Molecular Biology

Tuesday, February 22nd 2022 • 1:00 PM EST Registration (required): go.rutgers.edu/l6tcjpsx

LEARNING OBJECTIVES

This Institute for Quantitative Biomedicine Crash Course is a programming workshop designed to introduce life scientists to the power and flexibility of solving problems with Python. It is designed to move users beyond a "plug-and-play" approach that is based on spreadsheets and web applications in their teaching and research to writing scripts to parse large collections of data and to perform dynamic calculations. The live-coding workshop is designed to introduce specific coding skills, as well as provide insight into the broader array of open-access resources and libraries that are available for scientific computation.

Each live coding segment will be followed by a hands-on programming exercise to introduce you to the programming language and to help you identify the challenges associated with coding. You will learn to extract data from PDB files, first by working with one file to learn one set of tools, then by using a different set of tools to explore, sort and output results from a large number of files.

For those who are interested, a 12-hour workshop will be offered in July, 2022.

CO-ORGANIZERS:

Paul A. Craig, Ph.D., Professor of Biochemistry RIT Rochester Institute of Technology

Jessica A. Nash, Ph.D., Software Scientist Molecular Sciences Software Institute ^wRIT Molssi

CO-SPONSORS:



RCSB Protein Data Bank rcsb.org



Institute for Quantitative Biomedicine (IQB) iqb.rutgers.edu

PROGRAM

1:00-1:05 PM	Introduction Stephen K. Burley, M.D., D.Phil.: Founding Director, Institute for Quantitative Biomedicine, Rutgers University
1:05–1:10 PM	Welcome and Crash Course Learning Objectives Paul A. Craig, Ph.D., Professor of Biochemistry, Rochester Institute of Technology
	Jessica A. Nash, Ph.D., Software Scientist, Molecular Sciences Software Institute
1:10-2:00 PM	Lesson 1: Introduction to Python and to Jupyter Notebooks Paul A. Craig
2:00-2:10 PM	<i>Hands-on Exercise 1</i> Paul A. Craig and Jessica A. Nash
2:10-2:20 PM	Questions and Answers about Exercise 1
2:20-3:00 PM	<i>Lesson 2: Reading and Writing Files</i> Jessica A. Nash
3:00–3:10 PM	<i>Hands-on Exercise 2</i> Jessica A. Nash and Paul A. Craig
3:10-3:20 PM	Questions and Answers about Exercise 2
3:20-3:30 PM	Break
3:30-4:00 PM	<i>Processing Multiple Files</i> Paul A. Craig
4:00-4:20 PM	<i>Hands-on Exercise 3</i> Paul A. Craig and Jessica A. Nash
4:20-4:50 PM	<i>Visualizing structures in the Jupyter Notebooks</i> Jessica A. Nash
4:50-5:00 PM	Hands-on Exercise 4
5:00 PM	Closing Remarks and Acknowledgments Stephen K. Burley

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VIRTUAL CRASH

COURSE