BIOGRAPHICAL SKETCH

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NAME: Craig, Paul

eRA COMMONS USER NAME (credential, e.g., agency login): pcraig

POSITION TITLE: Professor

EDUCATION/TRAINING *(Begin with baccalaureate or other initial professional education, such as nursing, include postdoctoral training and residency training if applicable.)*

INSTITUTION AND LOCATION	DEGREE (if applicable)	START DATE MM/YYYY	END DATE MM/YYYY	FIELD OF STUDY
Oral Roberts University, Tulsa, OK	BS	09/1975	05/1979	Chemistry
The University of Michigan, Ann Arbor, Michigan	PHD	09/1979	05/1985	Biological Chemistry
Henry Ford Hosptial, Detroit, Michigan	Postdoctoral Fellow	03/1985	08/1988	Physical biochemistry of blood clotting

A. Personal Statement

My formal training is in biochemistry and I have skills in communicating with computer scientists. While I am not a programmer, I consider myself a computational biochemist and that is my research focus - developing computational tools to explore protein structure and function, then implementing them for researchers ranging from students to professionals. A summer research project at Brookhaven National Labs led to collaboration with Herbert Bernstein, which has resulted in the development of the ConScript [Mottarella, 2010] and ProMOL [Hanson, 2014] plugins for PyMOL. This has continued for 10 years, most recently in two 2015 manuscripts, “Annotation of Proteins of Unknown Function: Initial Enzyme Results“ [McKay T, 2015] and "Automated protein motif generation in the structure-based protein function prediction tool ProMOL" [Osipovitch, 2015]. Herbert is a mathematician and computer scientist with extensive experience in structural biology and biological databases. I combine a biological and functional perspective with many years of experience in the use and development of software. Our complementary skill sets have led to a fruitful collaboration that has been highly beneficial to students on both campuses. On a personal level, I find great fulfillment in having published six manuscripts that included 25 undergraduate student authors, as well as six manuscripts with five different pre-tenure faculty members.

1. Osipovitch M, Lambrecht M, Baker C, Madha S, Mills JL, Craig PA, Bernstein HJ. Automated protein motif generation in the structure-based protein function prediction tool ProMOL. J Struct Funct Genomics. 2015 Dec;16(3-4):101-11. PubMed PMID: 26573864; PubMed Central PMCID: PMC4684744.
2. McKay T, Hart K, Horn A, Kessler H, Dodge G, Bardhi K, Bardhi K, Mills JL, Bernstein HJ, Craig PA. Annotation of proteins of unknown function: initial enzyme results. J Struct Funct Genomics. 2015 Mar;16(1):43-54. PubMed PMID: 25630330; PubMed Central PMCID: PMC4332402.
3. Hanson B, Westin C, Rosa M, Grier A, Osipovitch M, MacDonald ML, Dodge G, Boli PM, Corwin CW, Kessler H, McKay T, Bernstein HJ, Craig PA. Estimation of protein function using template-based alignment of enzyme active sites. BMC Bioinformatics. 2014 Mar 27;15:87. PubMed PMID: 24669788; PubMed Central PMCID: PMC4229977.
4. Mottarella SE, Rosa M, Bangura A, Bernstein HJ, Craig PA. Conscript: RasMol to PyMOL script converter. Biochem Mol Biol Educ. 2010 Nov;38(6):419-22. PubMed PMID: 21567873; PubMed Central PMCID: PMC3134254.

B. Positions and Honors

Positions and Employment

1988 - 1993	Analytical Biochemist, BioQuant, Ann Arbor, MI
1993 - 1999	Assistant Professor, Rochester Institute of Technology, Dept. of Chemistry, Rochester, NY
1999 - 2003	Associate Professor, Rochester Institute of Technology, Dept. of Chemistry, Rochester, NY
2001 - 2002	Visiting Scholar, UCSD, San Diego Supercomputing Center, San Diego, CA
2003 -	Professor, Rochester Institute of Technology, Dept. of Chemistry, Rochester, NY
2011 - 2012	Associate Head, Rochester Institute of Technology, Dept. of Chemistry, Rochester, NY
2012 -	Head, Rochester Institute of Technology, School of Chemistry & Materials Science, Rochester, NY

Other Experience and Professional Memberships

1976 -	Member, American Chemical Society
1993 -	Member, American Society for Biochemistry & Molecular Biology
2007 -	Member, American Crystallographic Association

Honors

1979	National Merit Scholar, National Merit Scholar Corporation
1986	Fellow, American Heart Association
2017	Chemical Pioneer Award, American Institute of Chemists

C. Contribution to Science

1. Software Development and Implementation in Computational Biochemistry

   Since 1993, I have worked with students and faculty members on projects at the interface between life science and computer science programs. In 2004, our group at RIT began studying 3D modeling of macromolecules with PyMOL. Undergraduates from RIT then wrote the EZ-Viz plugin for PyMOL [Grell, 2006] to overcome the steep learning curve for PyMOL. This led to a collaboration with Herbert Bernstein that has resulted in the creation of a script convertor that allows PyMOL to accept Jmol/RasMOL scripts in the PyMOL command line [Mottarella, 2010]. Subsequently, our students developed ProMOL to help people propose protein function based on comparison to a series of active site templates [Hanson, 2014]. Recently, one of our M.S. students enhanced ProMOL to include automated motif generation [Osipovitch, 2015].

   a. Osipovitch M, Lambrecht M, Baker C, Madha S, Mills JL, Craig PA, Bernstein HJ. Automated protein motif generation in the structure-based protein function prediction tool ProMOL. J Struct Funct Genomics. 2015 Dec;16(3-4):101-11. PubMed PMID: 26573864; PubMed Central PMCID: PMC4684744.
   b. Hanson B, Westin C, Rosa M, Grier A, Osipovitch M, MacDonald ML, Dodge G, Boli PM, Corwin CW, Kessler H, McKay T, Bernstein HJ, Craig PA. Estimation of protein function using template-based alignment of enzyme active sites. BMC Bioinformatics. 2014 Mar 27;15:87. PubMed PMID: 24669788; PubMed Central PMCID: PMC4229977.
   c. Mottarella SE, Rosa M, Bangura A, Bernstein HJ, Craig PA. Conscript: RasMol to PyMOL script converter. Biochem Mol Biol Educ. 2010 Nov;38(6):419-22. PubMed PMID: 21567873; PubMed Central PMCID: PMC3134254.
   d. Grell L, Parkin C, Slatest L, Craig PA. EZ-Viz, a tool for simplifying molecular viewing in PyMOL. Biochem Mol Biol Educ. 2006 Nov;34(6):402-7. PubMed PMID: 21638731.

2. Biochemistry Education

   Early in my RIT career, I was tasked with creating an updated biochemistry lab. I received NSF support for this effort, primarily because of mentoring by Chris Rollman, who offered significant guidance as I prepared

the proposal. This led to my first publication at RIT [Craig, 1999]. Since that time, I have been heavily engaged in the use and development of molecular visualization software [Grell, 2006]. Among my most memorable experiences was my 2001-2002 sabbatical with Philip Bourne, who was an associate director of the Protein Data Bank at that time. Since then I have given invited talks at ACS and ASBMB conferences and recently led a workshop on the assessment of student learning with molecular visualization at a 2013 ASBMB conference, “Transforming Undergraduate Education in Molecular Life Sciences”. I am grateful to Jenny Loertscher for the invitation and her very helpful guidance on running a dynamic, interactive workshop. A collaboration that focused on developing a rubric for student learning with molecular visualization has developed from this workshop and is starting to have an impact on many campuses [Dries, 2016]. Currently I lead the BASIL team (Biochemistry Authentic Science Inquiry Lab; basiliuse.blogspot.com), which is promoting implementation of a Course-based Undergraduate Research Experience (CURE) focused on prediction of protein function [Craig, 2017].One of my proudest moments occurred at the 2015 ASBMB meeting when one of my undergraduates gave an invited talk.

a. Craig PA. A survey on faculty perspectives on the transition to a biochemistry course-based undergraduate research experience laboratory. Biochem Mol Biol Educ. 2017 Apr 16;PubMed PMID: 28419715.
b. Dries DR, Dean DM, Listenberger LL, Novak WR, Franzen MA, Craig PA. An expanded framework for biomolecular visualization in the classroom: Learning goals and competencies. Biochem Mol Biol Educ. 2017 Jan 2;45(1):69-75. PubMed PMID: 27486685; PubMed Central PMCID: PMC5297871.
c. Grell L, Parkin C, Slatest L, Craig PA. EZ-Viz, a tool for simplifying molecular viewing in PyMOL. Biochem Mol Biol Educ. 2006 Nov;34(6):402-7. PubMed PMID: 21638731.
d. Craig PA. A Project Oriented Biochemistry Laboratory Course. Journal of Chemical Education. 76(8):1130.

3. Classical Enzymology

I received my Ph.D. in Biological Chemistry with Eugene E. Dekker (who earned his Ph.D. with William C.M. Rose), where we focused on enzymology and protein chemistry of amino acid metabolism [Craig, 1986]. At that time, I developed an interest in chromatography, enzyme kinetics, and chemical modification of enzyme. I was also fascinated by the role of metal ions in protein structure and function [Craig, 1990]. My post-doctoral training was in the physical biochemistry of blood clotting with Joseph D. Shore and Steven T. Olson. I studied enzyme kinetics with factor Xa (a serine protease) in its interactions with antithrombin III and heparin using traditional UV-Visible spectroscopy as well as fluorescence, including stopped flow methods [Craig, 1989; Olson, 1992].

a. Craig PA, Dekker EE. L-threonine dehydrogenase from Escherichia coli K-12: thiol-dependent activation by Mn2+. Biochemistry. 1986 Apr 22;25(8):1870-6. PubMed PMID: 3518793.
b. Craig PA, Olson ST, Shore JD. Transient kinetics of heparin-catalyzed protease inactivation by antithrombin III. Characterization of assembly, product formation, and heparin dissociation steps in the factor Xa reaction. J Biol Chem. 1989 Apr 5;264(10):5452-61. PubMed PMID: 2925612.
c. Craig PA, Dekker EE. The sulfhydryl content of L-threonine dehydrogenase from Escherichia coli K-12: relation to catalytic activity and Mn2+ activation. Biochim Biophys Acta. 1990 Jan 19;1037(1):30-8. PubMed PMID: 2104757.
d. Olson ST, Björk I, Sheffer R, Craig PA, Shore JD, Choay J. Role of the antithrombin-binding pentasaccharide in heparin acceleration of antithrombin-proteinase reactions. Resolution of the antithrombin conformational change contribution to heparin rate enhancement. J Biol Chem. 1992 Jun 25;267(18):12528-38. PubMed PMID: 1618758.

4. Analytical Biochemistry and Proteomics

I spent five year at a startup company in Ann Arbor, MI, called BioQuant, where we studied noninvasive detection of small molecules in alternative body fluids, including the analysis of cocaine metabolites in blood, urine and saliva [Schramm, 1993]. I also gained experience with synthesis of labeled bioconjugates for use in immunoassays [Schramm, 1990]. When I moved to academia, I became interested in

proteomics, which led to an article about proteomics for undergraduates [Kim, 2010] and a simulation of 2D electrophoresis and Tandem MS, which provides undergraduates with training with technology that their institutes may not be able to afford [Fisher, 2012].

a. Schramm W, Smith RH, Jackson TM, Craig PA, Grates HE, Minton LL. Rapid solid-phase immunoassay for 6-keto prostaglandin F1 alpha on microplates. Clin Chem. 1990 Mar;36(3):509-14. PubMed PMID: 2311222.
b. Schramm W, Craig PA, Smith RH, Berger GE. Cocaine and benzoylecgonine in saliva, serum, and urine. Clin Chem. 1993 Mar;39(3):481-7. PubMed PMID: 8448861.
c. Kim TD, Craig PA. Introducing proteomics in the undergraduate curriculum: A simple 2D gel electrophoresis exercise with serum proteins. Biochem Mol Biol Educ. 2010 Jan;38(1):29-34. PubMed PMID: 21567787.
d. Fisher A, Sekera E, Payne J, Craig P. Simulation of two dimensional electrophoresis and tandem mass spectrometry for teaching proteomics. Biochem Mol Biol Educ. 2012 Nov-Dec;40(6):393-9. PubMed PMID: 23166029.

D. Additional Information: Research Support and/or Scholastic Performance

Ongoing Research Support

1709170, NSF DUE-IUSE. Craig, Paul (PI). 09/01/17-08/31/20
Title: Collaborative Research: Using protein function prediction to promote hypothesis-driven thinking in undergraduate biochemistry education
Summary: This is a proposal for the second phase of a project bringing authentic research experiences into undergraduate biochemistry lab courses as Course-based Undergraduate Research Experiences (CUREs). In the first phase of this project, students on six campuses have been participating in authentic research experiences, integrating computational ("in silico") and wet lab ("in vitro") techniques as they characterize proteins whose 3D structures are known but to which functions have not been previously ascribed. Changes in faculty and teaching assistant competence are also being evaluated for (1) effective teaching with structural biology tools, (2) the development of skills in the area of measuring learning gains by students, and (3) their perceptions of CURE-like teaching approaches. In the second phase of this project, students' learning and their growth as scientists will be assessed by local biochemistry faculty and evaluated by Purdue University education researchers, in terms of students' understanding of research methods, visualization, biological context, and mechanisms of protein function.

1503811, NSF DUE-IUSE-Engaged Student Learning: Exploration. Craig, Paul (PI). 06/01/15-05/31/18
Title: Collaborative Research: Using protein function prediction to promote hypothesis-driven thinking in undergraduate biochemistry education
Summary: Students on six campuses (California Polytechnic San Luis Obispo, Hope College, Oral Roberts University, Rochester Institute of Technology, St. Mary's University, and Ursinus College) will participate in authentic research experiences in their undergraduate biochemistry lab courses. They will integrate computational ("in silico") and wet lab ("in vitro") techniques as they characterize proteins whose three dimensional structures are known but to which functions have not been previously ascribed. Their learning as students and their growth as scientists will be assessed in terms of research methods, visualization, biological context, and mechanism of protein function.

Completed Research Support

2R15GM078077-02, NIH. Craig, Paul (PI). 09/01/11-08/31/15
Title: Algorithmic assignment of probable function to proteins of previously unknown function
Objectives and Specific Aims: The goal of this project is to extend and apply algorithms that show promise in assigning a probable function for PDB entries of currently unknown function. This should contribute to deriving

benefit from the Protein Structure Initiative by "help[ing] researchers illuminate structure-function relationships and thus formulate better hypotheses and design better experiments." Research Design and Methods: There are currently 2939 entries in the Protein Data Bank with the classification "Unknown Function". We have developed a software plug-in for the PyMOL molecular graphics environment called ProMOL that relies on the geometric relationships conserved in enzyme catalytic sites. Motifs in ProMOL were created from the active site specifications found in the Catalytic Site Atlas (CSA) (http://www.ebi.ac.uk/thornton-srv/databases/CSA/). Our approach explicitly searches for CSA- defined catalytic site residues according to specific atomic geometry. This dispenses with the need to filter out confounding elements such as conserved folding domains or ligand binding regions. We will extend the number of motifs in ProMOL's Motif Finder, using both newly created ProMOL motifs to include representatives from the most prominent protein families, increase automation of the process and then evaluate all PDB entries described as having "unknown function". Both software and results will be openly released to the community.

3R15GM078077-02S3, NIH. Craig, Paul (PI). 08/08/14-08/31/15
Algorithmic assignment of probable function to proteins of previously unknown function
Supplement to NIH Award 2R15GM078077-02

3R15GM078077-02S1, NIH. Craig, Paul (PI). 11/14/11-08/31/14
Algorithmic assignment of probable function to proteins of previously unknown function
Supplement to award 2R15GM078077-02

3R15GM078077-02S2, NIH. Craig, Paul (PI). 12/19/13-08/31/14
Algorithmic assignment of probable function to proteins of previously unknown function
Supplement to NIH Award 2R15GM078077-02

1R15GM078077-01, NIH. Craig, Paul (PI). 07/01/06-06/30/10
Title: Structural Biology Extensible Visualization Scripting Language
Summary: The goal of the SBEVSL project is to create a new extensible scripting language for molecular graphics, as used in structural biology, by combining the intiutive expressive power of the widely used scripting language created by Roger Sayle for RasMol with the general object-oriented extensibility of the Python scripting of PyMOL. Major existing open source molecular graphics programs, including RasMol, Jmol and PyMol will be adapted to accept scripts written in the new scripting language. In addition, use of command languages for visualization in structural biology yields precise control and reproducibility not obtainable by users with an ordinary pointing device such as a mouse or a dial box. The SBEVSL project will extract all the concepts used in the command languages of major molecular graphics programs and gather them in one master ontology, using this essential dictionary as a relational database with CIF. Defining SBEVSL in terms of the dictionary and UML will allow expression of scripts in multiple formats so that SBEVSL can be widely used.

3R15GM078077-01S1, NIH. Paul Craig (PI). 04/27/09-06/30/10
SBEVSL - Structural Biology Extensible Visualization Scripting Language
Supplement to NIH Award 1R15GM078077-01

DUE-0402408, NSF. Craig, Paul (Co-PI). 02/01/04-01/31/07
Building a Cross-Institutional Collaboratory for 3D Visualization in Technical Education and Training
The NSF ATE program supported a joint program between Brookhaven National Lab and several community colleges and PUIs. The focus was on using 3D visualization for training the workforce. Projects included architecture, biochemistry, and engineering.