

Jordan R. Willis

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PROFILE

Computational and molecular biologist working in the area of human antibodies and vaccines

- 8 years experience with molecular biology
- 4 years experience with cell culture and transfection
- 5 years experience with molecular modeling
- 3 years experience with high throughput sequencing and analysis

EDUCATION

Vanderbilt University Medical Center, Nashville, TN 2008-present

Ph.D. Chemical and Physical Biology, defense anticipated November 2013.

Dissertation: "Rational Antibody Design: From Mechanisms of Antibody Binding to Novel Vaccine Strategies"

Advisors: James E. Crowe, Jr., M.D., Jens Meiler Ph.D.

Northwest Missouri State University 2008

Bachelor of Science in A.C.S Accredited Chemistry

Magna Cum Laude, In Honors

GPA 3.81/ 4.0

Northwest Missouri State University 2008

Bachelor of Arts in Biology, with a focus in Molecular Biology

Magna Cum Laude, In Honors

GPA 3.81/ 4.0

RESEARCH EXPERIENCE

Vanderbilt Vaccine Center, Center for Structural Biology,

Vanderbilt University

Graduate Student

2008-present

Principal Investigators: James E. Crowe, Jr., M.D, Jens Meiler Ph. D.

My project involved using computational design to answer specific questions in

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immunology, with a focus on antibody design. The computational work was accomplished in the Meiler laboratory while the experimental laboratory work was conducted in the Crowe laboratory. My thesis work can be divided into four parts: 1) Multi-state antibody design to interrogate mechanisms for antibody polyspecificity. How do antibodies use a limited sequence repertoire to bind many antigens? 2) Molecular mechanisms of CD4-binding site escape for HIV-1 gp120. How does gp120 escape neutralization by VRC01 and b12, two broadly neutralizing antibodies that bind the CD4-binding site? We used computational characterization, homology modeling, and biophysical characterization to test our hypothesis. 3) HIV broadly neutralizing antibody design from HIV-naïve donor sequences. Using computational modeling, high-throughput sequencing, and bioinformatics tools, we developed antibodies designed from HIV-naïve donor sequence pools that mimic broadly neutralizing antibodies with exceptionally long HCDR3s. The goal of this project is to see how close HIV-naïve individuals are to development of broadly neutralizing antibodies with long HCDR3s against HIV. 4) Using multi-state design to broaden reactivity of binding of influenza the HA stem binding antibody CR6261 to the stem of HA in virus subtypes that CR6261 did not naturally bind.

Department of Chemistry, University of Missouri

2007-2008

Principal Investigator: Kent Gates, Ph. D.

Lead optimization drug discovery of hypoxic molecules that target tumors. Using the pharmacophore Tirapazamine as a scaffold, I used combinatorial synthesis techniques to add organic groups and evaluate structural activity relationships.

SPECIALIZED TECHNICAL EXPERTISE

- Molecular Modeling
 - Development and application of the software suite Rosetta
 - Molecular mechanics applications with software suite MOE and AMBER
 - Molecular viewing, PyMOL and RasMoL
- Bioinformatics resources and tools
 - Proteomics
 - Protein structure prediction
 - Post-translational modifications
 - Similarity search and alignments
 - Phylogeny and evolution
- Dynamic computer languages
 - Java
 - C++
 - Scripting with Python and BioPython
 - BioPython development
- Computer databases
 - MySQL
 - MongoDB

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- Influenza and human immunodeficiency virus (HIV) applications
 - HIV neutralization assays
- Virus-like particles and pseudovirions
 - Production and purification
- Viral pathogenesis
- Protein expression and purification
 - Novel cloning strategies
 - Novel purification strategies
 - Cell culture and maintenance
- Biophysical characterization
 - Biolayer interferometry
 - ELISA
 - Isothermal titration calorimetry

RESEARCH PUBLICATIONS

1. Joyner AS, **Willis JR**, Crowe JE Jr, Aiken C (2011) Maturation-induced cloaking of neutralization epitopes on HIV-1 particles. ***PLoS Pathog*** 7(9): e1002234.
2. Briney BS, **Willis JR**, Crowe JE Jr (2012) Human peripheral blood antibodies with long HCDR3s are established primarily at original recombination using a limited subset of germline genes. ***PLoS ONE*** 7(5): e36750
3. Briney BS, **Willis JR**, McKinney BA, Crowe JE (2012) High-throughput antibody sequencing reveals genetic evidence of global regulation of the naïve and memory repertoires that extends across individuals plasticity ***Genes and Immunity*** 13(6), 469-473.
4. Briney BS, **Willis JR**, Crowe JE (2012) Location and length distribution of somatic hypermutation-associated DNA insertions and deletions reveals regions of antibody structural plasticity ***Genes and Immunity*** 13(7), 523-529
5. Briney BS, **Willis JR**, Hicar MD, Thomas JW, Crowe JE (2012) Frequency and genetic characterization of V(DD)J recombinants in the human peripheral blood antibody repertoire. ***Immunology*** 131(1) 56-64
6. **Willis JR**^{*}, Combs SA^{*}, DeLuca SL^{*}, DeLuca SH^{*}, Lemmon GH^{*}, Nguyen ED^{*}, Sheehan JH, Nannemann DP, Meiler J (2013) Comparative modeling and small-molecule ligand docking in Rosetta. ***Nature Protocols*** 8(7) 1277-1298
7. **Willis, JR**, Briney, B. S., Deluca, S. L., Crowe, J. E. & Meiler, J. (2013) Human germline antibody gene segments encode polyspecific antibodies ***PLoS Computational Biology*** 9, e10030 AA45 L

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In submission or preparation

1. Briney, BS, **Willis JR**, Finn, JA, McKinney, BA, Crowe JE (2013) Tissue-specific expressed antibody variable gene repertoires. **PLoS One**
2. **Willis JR**, Finn, JA, Briney, BS, Meiler J, Crowe, JE (2013) HIV-neutralizing long heavy chain complementary determining region 3 sequences from HIV-naïve donors, in preparation.
3. **Willis JR**, Meiler J, Crowe JE Entropic mechanisms of neutralization escape of CD4 binding site-targeted antibodies predicted using Rosetta, in preparation.
4. **Willis JR***, Nannemann DP*, Cisneros A, Meiler J, Crowe JE Cross sub-group binding influenza antibodies designed with Rosetta, in preparation.

TEACHING EXPERIENCE

Instructor - Rosetta teaching workshop Developed protocol, taught background and gave hands-on demonstration for design for Rosetta teaching workshop 2012	2012
Instructor - Rosetta teaching workshop Developed protocol, taught background and gave hands-on demonstration for protein docking for Rosetta teaching workshop 2011	2011
Laboratory teaching assistant to Professor Richard Toomey, Northwest Missouri State University Chemistry 1 and 2	2007-2008
Tutor - Talent Development Center, Northwest Missouri State University Tutored in the following subjects. General physics I and II. General, organic, analytical and physical chemistry. All mathematics including statistics, algebra, and calculus.	2005-2006

HONORS AND AWARDS

Research and Scholarly Awards

NIH 5 T23 AI060571 HIV/AIDS Research Training Program Vanderbilt University	2010-2011
Steven's Research Scholarship, \$4,800	2007-2008

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University of Missouri

Mary Marie Smith Chemistry Scholarship, \$4,850/year Northwest Missouri State University	2007-2008
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J. Gordon Strong Chemistry Scholarship, \$2,450/year Northwest Missouri State University	2006-2007
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Tower Scholar, \$1,500/year Northwest Missouri State University	2004-2008
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Travel Awards

Keystone HIV Vaccine Symposium Scholarship	2012
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Chemical and Physical Biology Travel Award	2012
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IBC Antibody Engineering Symposium Scholarship	2011
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RECENT ASSIGNED TRAINEES (Under the mentorship of laboratory PI)

1. Albert Cisneros Graduate student, Crowe laboratory	2013
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2. Martha Wall Graduate student, Young laboratory, Vanderbilt University	2012
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3. Katherine Bradley MPH student, University of California Berkeley	2012
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4. Jessica Finn Graduate student, Crowe laboratory	2011
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5. Mason Sanders Summer undergraduate research intern	2011
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6. Katherine Nichols Graduate student, Kalams laboratory, Vanderbilt University	2010
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ABSTRACTS AND PRESENTATIONS (underline indicates presenter)

1. Willis JR, Crowe JE, Meiler J (2013) Broadly neutralizing antibodies to HIV in HIV-naïve donors populations: The broadly neutralizing antibody problem. Chemical and physical biology retreat

2. Finn, JA, Nannemann, DP, **Willis JR**, Crowe, JE Jr (2013) *De novo* modeling of antibody CDRH3 loops with constraints. RosettaCon
 3. **Willis JR**, Briney BS, Finn J, Meiler J, Crowe JE Jr (2012) Potential paradigm shifts in HIV vaccine design using ultra high-throughput sequencing and antibody modeling. Chemical and physical biology retreat
 4. Briney BS, **Willis JR**, Crowe JE Jr (2012) Somatic hypermutation-associated insertions and deletions reveal regions of antibody structural plasticity. Keystone symposium on HIV vaccines
 5. Finn JA, **Willis JR**, Briney, BS, Crowe, JE Jr, Meiler J (2012) Structural prediction of long complementarity determining region 3 loops. RosettaCon
 6. Briney BS, **Willis JR**, Crowe JE Jr (2011) Genetic and functional analysis of the human anti-HIV antibody repertoire. Keystone symposium on HIV vaccines
 7. Briney BS, **Willis JR**, Crowe JE Jr (2011) Genetic origin of long HCDR3s in the circulating antibody repertoire. IBC life sciences - Antibody engineering & therapeutics
 8. **Willis JR**, Crowe JE Jr, Meiler J (2011) Structural basis for development of broadly neutralizing antibodies to HIV using computational predictions. Chemical and physical biology retreat.
 9. **Willis JR**, Briney BS, Crowe JE Jr, Meiler J (2011) Antibody design infers optimal sequences for binding breadth and affinity maturation. IBC life sciences - Antibody engineering & therapeutics
 10. **Willis JR**, Crowe JE Jr, Meiler J (2010) Constrained design of broadly neutralizing HIV antibody-antigen interactions. RosettaCon
 11. **Willis JR**, Meiler J, Crowe JE Jr (2009) HIV gp-160 targeted broadly neutralizing antibodies - modeling and design. RosettaCon
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INVITED LECTURES AND SEMINARS

Willis JR, Finn JA, Briney BS, Meiler J, Crowe JE Jr (2012) Potential paradigm shifts in vaccine design using Rosetta. RosettaCon

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Willis JR, Briney BS, Meiler J, Crowe JE Jr (2012) Structure analysis of healthy donor repertoire confers sequences that match long complementary determining regions of broadly neutralizing antibodies. Keystone symposium on HIV vaccines

Willis JR, Crowe JE Jr, Meiler J (2011) Multi-state design of antibody-antigen interactions confers conformational flexibility. RosettaCon

MEMBERSHIPS

American Society of Collegiate Scholars	2004–2008
American Chemical Society	2006-2010
Tri-Beta, Biology Honor Society	2008

REFERENCES

1. James E. Crowe, Jr. MD
Ann Scott Carell Chair
Professor Pediatrics and Microbiology and Immunology
Director, Vanderbilt Vaccine Center
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3. Kent S. Gates, Ph.D.
Herman G. Schlundt Distinguished Professor of Chemistry
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