

## CURRICULUM VITAE Yuhua Song, Ph.D.

Professor (with tenure) in Department of Biomedical Engineering  
The University of Alabama at Birmingham  
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### Research Statement

My research group uses integrated multiscale computational modelling and experimental approaches to investigate the structural, molecular and functional mechanisms of the biomolecular interactions. Our goal is to identify endogenous and exogenous small molecules, including repositioning of FDA-approved drugs, to regulate the biomolecular interactions underlying important cellular activities in Alzheimer's disease, cancer, cardiovascular disease, dermatopathology, regenerative medicine and precision medicine, with current focus in Alzheimer's disease, for potential therapeutic treatment. Methodology development for multiscale modelling of complex biological systems continues to be a focus of my research group. Our research program is currently funded by NIH R01, NSF, Alzheimer's Drug Discovery Foundation and UAB internal grants.

### Education Statement

My goals for education are to inspire the students' interest, motivate students to actively think and be committed in the course and research, teach students to critically read literatures, and help the students to develop critical and independent thinking, problem solving and team working skills, and good working ethic that are important for the students' future academic and professional development. I have mentored more than 50 trainees with 15 minority and 19 female trainees since I joined UAB in 2006, including postdoctoral associates, graduate, undergraduate and high school students, research scholars, and research assistants. The trainees in my research group have been productive and are recognized by students' awards. Due to my dedication to mentees' training, I was awarded Graduate Dean's Excellence in Mentorship Award.

### Education and Training

1985 - 1989	B.S. in Materials Science and Eng., Jilin University of Technology, Jilin, China
1993 - 1996	M.S. in Materials Science and Eng., Harbin University of Sci and Tech, Harbin, China
1996 - 1998	Ph.D. in Materials Science and Eng., Harbin Institute of Technology, Harbin, China
1998 - 2001	Post-Doc in Computational Mechanics, Tsinghua University, Beijing, China
2001 - 2002	Post-Doc in Computational Biomechanics, University of Pittsburgh, Pittsburgh, PA
2002 - 2005	Post-Doc in Computational Biology, Washington University in St. Louis, St. Louis, MO
2013 - 2016	Master of Business Administration, University of Alabama at Birmingham

### Academic Appointments

2022 –	Professor with Tenure, Department of Biomedical Engineering, The University of Alabama at Birmingham (UAB)
2012 - 2022	Associate Professor with Tenure, Department of Biomedical Engineering, UAB
2006 - 2012	Assistant Professor, Department of Biomedical Engineering, UAB
2005 - 2006	Research Instructor with Dr. Nathan A. Baker, Center for Computational Biology Dept. of Biochemistry and Molecular Biophysics, Washington University in St. Louis
2002 - 2005	Research Associate with Dr. Nathan A. Baker, Center for Computational Biology Dept. of Biochemistry and Molecular Biophysics, Washington University in St. Louis
2001 - 2002	Postdoctoral Fellow with Dr. Savio L-Y. Woo, Musculoskeletal Research Center, Dept. of Orthopedic Surgery, University of Pittsburgh
1998 - 2001	Postdoctoral Fellow with Dr. Yongnian Yan

Center for Laser Rapid Forming & Bio-Manufacturing Engineering,  
Dept. of Mechanical Engineering, Tsinghua University, China

### Other University Affiliations/Positions at UAB

2022 - present Scientist, Center for Clinical and Translational Science (CCTS), UAB  
2021 - present Scientist, Center for Neurodegeneration and Experimental Therapeutics, UAB  
2011 - present Faculty of Structural Biology Program, UAB  
2011 - present Member, Center for Nanoscale Materials and Biointegration, UAB  
2010 - present Faculty of Graduate Biomedical Science, UAB  
2009 - present Associate Scientist, UAB Comprehensive Cancer Center, UAB  
2007 - present Secondary Faculty, Department of Biochemistry and Molecular Genetics, UAB  
2007 - present Faculty of Medical Scientist Training Program, UAB  
2006 - present Associate Scientist, Center for Computational and Structural Dynamics, Center for Structural Biology, UAB  
2006 - present Associate Scientist, Center for Metabolic Bone Disease, UAB  
2006 - present Associate Scientist, BioMatrix Engineering and Regenerative Medicine Center, UAB  
2011 - 2012 Associate Director, Center for Computational and Structural Dynamics, UAB

### Awards and Honors

2021 – 2026 NIH R01 Award from National Institute on Aging  
2021 NSF-supported XSEDE XRAC award  
BIO200050 (computational resources)  
2020 - 2021 COVID-19 HPC Consortium Award spearheaded by White House of Sci and Tech Policy, U.S. Dept of Energy, NSF and IBM (TG-BIO200084, computational resources)  
2020 – 2021 NSF-supported XSEDE award  
MCB200181 (computational resources)  
2017 Graduate Dean's Excellence in Mentorship Award for 2017  
2013 NSF-supported XSEDE award  
MCB130041 (computational resources)  
2012 - 2018 NSF award from Biomedical Engineering Program in Division of Chemical, Bioengineering, Environmental, and Transport Systems at NSF  
2012 – 2013 NSF-supported Extreme Science and Eng Discovery Environment (XSEDE) award  
MCB130026 (computational resources)  
2009 - 2015 NIH K25 Mentored Quantitative Research Career Development Award, NIH/NCI  
2008 - 2009 Startup/Educational Allocation award for computational resources  
NSF's Partnerships for Advanced Computational Infrastructure  
2008 - 2009 The Development Allocation Committee Award for computational resources  
NSF's Partnerships for Advanced Computational Infrastructure  
2007 - 2008 UAB ADVANCE Faculty Research Awards through the sponsorship of NSF  
2006 - 2007 Medium Resource Allocations Committee Award for computational resources  
NSF's Partnerships for Advanced Computational Infrastructure  
2005 - 2006 Development Allocations Committee Award for computational resources  
NSF's Partnerships for Advanced Computational Infrastructure  
2002 Scholarship for the Grace Hopper celebration of women in computing  
2000 Postdoctoral Fellowship, China National Science Foundation

### Professional Affiliations

Biophysical Society      American Association for Cancer Research      American Chemical Society  
American Society for Biochemistry and Molecular Biology      American Heart Association  
Protein Society      National Center for Faculty Development & Diversity

### Further Career Development

2022 – present Leadership Development for Engineering Program Directors  
2021 Faculty Search Committee Training

- 2019 – present National Center for Faculty Development & Diversity, online career development and Mentoring resources: monthly webinars, multi-week courses etc.
- 2016 – present UAB Center for Teaching and Learning
- 2012 GRD 717 Course: Principles of Scientific Integrity
- 2010 Excellence in Teaching Seminar Series by the UAB Office for Faculty Development and Faculty Affairs
- 2009 – present Biohazard management, biosafety training from UAB Occupational Health and Safety department, Certificates for Working with Mice in Research and Using Animals for Teaching Testing and Research at UAB
- 2009 Teaching Portfolio Workshop
- 2008 - present Professional Development Seminar Series by UAB Center for Clinical and Translational Science
- 2006 Master Teacher Program

### Teaching Contribution (\* New courses development)

- \* BME 333 Biomechanics of Solids (Instructor), Spring 2008 – current, UAB
- \* BME 680/780 Biomolecular Modeling (Instructor), Fall 2015 – current, UAB
- BME 150 Computer Meth in EGR, Fall, 2013, UAB
- \* BME 480/580 Biomolecular Modeling (Instructor), Fall 2007, 2009, UAB
- BME 330 Biomechanics (Instructor), Spring 2007, UAB
- Lecture in “Mathematical Methods for Biophysics and Biochemistry (Bio-5329)” at Washington University in St. Louis
- Lab course development for “Modeling Biomolecular Systems II (BME-540)” at Washington University in St. Louis
- Advised graduate students, undergraduate and high school students at UAB, Washington University in St. Louis, University of Pittsburgh and Tsinghua University

### Educational Contribution

Current and past total students/trainees: 52 with 15 minority and 19 female trainees.

Table of current and past trainees with current position detailed in Appendix.

\* Minority student; \*\* female student

### Current Students/Trainees

#### Graduate students and research assistants

Rory A Greer (PhD) (Awardee of NIHT32 Training Grant; UAB Blazer Fellowship);

Hunter B Dean (PhD, MD) (jointly training with Dr. Erik Roberson.

Awardee of NIHT32 Training Grant in Neurodegeneration at UAB, 2019, 2020

Awardee of Alzheimer's of Central Alabama fellowship, 2021, 2022

Awardee of GSG Trainee Professional Development and Travel Award for *Society for Neuroscience meeting 2022*

Ryan A. Tuckey (PhD, MD) (jointly training with Dr. Erik Roberson)

Amanda M Plain\*, \*\* (PhD, part time);

Thi Kieu Duyen Tran \*\* (M.S.)

Urvi Rawal \*\* (M.S., rotation student)

#### Undergraduate students

Shalarrria Cooper\*, \*\*; Annabel Lynne Johnson\*\*, Van Winkle, Sarah Gabrielle

### Past Students/Trainees

#### Graduate students

Helen E Brinyark \*\* (PhD rotation, 2021 - 2022); Adam E Bashir (MD) (2018-2019);

Caleb M Graham (Master rotation, Fall 2019); Romone Fancy \* (PhD, graduated in Dec 2017);

Hongyi Yang \*\* (PhD, graduated in Dec 2015); Tiara Napier \*, \*\* (MS, graduated in 2013);

Di Pan (MS, graduated in 2009); Qi Yan (MS, graduated in 2009);  
Mohit A Limdi (PhD rotation, 2016 - 2017); AUFAN, Muhammad Rifqi (PhD rotation, 2017);  
Khanh T Nguyen\*\* (PhD rotation, Fall 2018); Molly Sears Buckley\*\* (MS rotation, Fall 2018)

#### Postdoctoral researcher, Research scholar and Research assistant

Yuwei Song \*\* (2019 – 2021); Justin L. Howell (2013 – 2016); Lingyun Wang (2011 – 2014);  
Qinghua Zeng (2014); Thomas Schmid (2012); Daixi Li (2009 – 2010);  
Huikuan Chao (2009 – 2010); Bibo Shi (2008 – 2009); Yuemin Liu (2006 – 2007)

#### Undergraduate students

Han Jing (2022); Hrithik Praveen (2019 – 2022); Kyla Alexsa Gabriel\*, \*\* (2019 – 2022); Jason Zhang  
(2020 – 2021), Zainab Ameir Ahmad \*\* (2018 – 2020); Patel, Kishan M (2018); Hong, Seoeui \*\*  
(2018); Vaishali Nijampatnam \*\* (2016-2017); Ruta Sanjay Bhat \*\* (2016-2017); Samuel Holder  
(2016); Nichelle Alyson Preston \*\* (2016); Dynisty Everette \* (2015); Julian Dill \* (2015); Brady  
Dulak (2014); Musa Williams \* (2012); Kevin J Anderson \* (2009 – 2011); Valentine Nwachukwu\*  
(2011); Jonathan Suever (2007 – 2008); Russell Green (2007 – 2008); Joseph C Pak (2008)

#### High school students

Amy Zhang \*\* (2016 – 2017, now at Harvard U); Courtney Mobbs \*\* (2016);  
James Browning (2014 – 2015, now at UAB); Brea Reese\*, \*\* (2013); Jarvis Williams \* (2011);  
Christopher Evans \* (now at UAB, 2010, 2011); Nichele Cantrell \*, \*\* (2009); Theodore Tolvin \* (2008)

#### **Student Thesis or Dissertation Committee**

LaBreesha Batey, Ph.D student (2022 - current); Ari Benjamin Ginsparg, Ph.D. student (2020 - current);  
Khanh T Nguyen, Ph.D. student (2021 - 2022); Cockrell, Benjamin Evan, B.S. (2021 - 2022);  
Susan Floyd, B.S. (2021 - 2022); Ji Hee Kim, Ph.D. candidate (2017 - 2021);  
Chidinma Anakwenze, B.S. (2010 – 2011); Cordero D. Core, Ph.D. candidate (2011 - 2013);  
Vinuta P Mayakonda, B.S. (2011 - 2012); Ian T Cook, Ph.D. (2009 - 2012);  
Kyle E Murdock, B.S. (2013); Hongyi, Yan, Ph.D. (2008 - 2014);  
Vinuta P Mayakonda, B.S. (2011 – 2012); David H. Johnson, Ph.D. (2008 - 2014);  
Amanda M Plain, Ph.D. candidate (2008 - 2016); Lurong Pan, Ph.D. (2009 - 2013);  
Chidinma Anakwenze, B.S. (2010 - 2011); Xin Chen, Ph.D. (2006 - 2008);  
Muhammad Y. Qadri, M.D, Ph.D. (2007 - 2009)

#### **Awards for Students**

Hunter B. Dean, MD/PhD student

- Awardee of NIH T32 Training Grant in Neurodegeneration at UAB, 2019, 2020
- Awardee of Alzheimer's of Central Alabama fellowship, 2021, 2022
- Awardee of GSG Trainee Professional Development and Travel Award for *Society for Neuroscience meeting 2022*

Rory A Greer, PhD student

- Awardee of UAB Blazer fellowship, 2021 – 2022
- Awardee of NIH T32 Training Grant at UAB, 2022-2024

Helen E Brinyark, PhD student

- Awardee of UAB Blazer Fellowship, 2021 - 2022

Jason Zhang, BME Undergraduate Student

- Honors College Presidential Summer Fellowship, 2020
- First Place, UAB Summer Research Expo, 2020
- UAB Undergraduate Student Government Association (USGA) travel grant, 2020
- Full scholarship from MIT biological engineering graduate program, 2021
- Tau Beta Pi Fellowship for graduate school study, 2021

Romone Fancy, M.S., PhD

- Graduate fellowship from The Comprehensive Minority Faculty and Student Development Program at UAB (2014–2017)
- NSF Bridge to the Doctorate fellowship from The Office for Equity and Diversity at UAB (2011–2013)
- AACR Minority Scholar in Cancer Research Award 2012
- First-Place for poster presentation in Biomedical Engineering Research Symposium at UAB, 2012

Tiara Napier, M.S.

- NSF Bridge to the Doctorate fellowship from The Office for Equity and Diversity at UAB (2011-2013)
- First-Place in the Engineering Category for poster presentation at conference for NSF Bridge to the Doctorate Fellows in Auburn, 2012

Kevin J Anderson, B.S.

Recognized in Sci and Tech Honors Program in its Spring Celebration of Excellence at UAB, 2011

Di Pan, B.S.

Ireland Tuition Scholarship, 2008-2009

Jonathan Suever, B.S.

The Mr. & Mrs. Kwok-Chong Woo Grant” from Orthopaedic Research Laboratory Alumni Council (2007–2008)

## **Department, School and University Service at UAB:**

### ***Department level service***

- Director for Graduate Program Committee, Department of Biomedical Engineering (BME) (2021 Summer – 2022 Summer) (recruitment of the largest group of incoming students in at least past six years)
- Associate Director for Graduate Program Committee, BME Department (2020 Fall - 2021 Spring)
- Graduate Program Committee, BME Department (2006 – 2013, 2016- present)
- Academic Research Excellence Committee, BME Department (2016 - 2020)
- Visibility & Recognition Committee, BME Department (2016 - 2020)
- BME Chair Search Committee (2015)
- Department Strategic Planning Committee, BME Department ( 2007 - 2009)

### ***School level service***

- Neuro-engineering Graduate Program Committee, School of Engineering (2020 – current)
- Neuro-engineering Faculty Search Committee (2020 – present)
- School’s representative on the UAB commission on the Status of Women (2020 - current)
- Academic Affairs Committee, School of Engineering (2018 - present)
- Quality Assessment Committee, School of Engineering, UAB (2014 - 2016)
- Faculty Advisor for Society of Women Engineers, School of Engineering (2011 - 2016)
- Faculty member for Society of Women Engineers, School of Engineering (2016 - present)
- Equity and Diversity Committee, School of Engineering (2007 - 2009)

### ***University level service***

- UAB President’s Commission on the Status of Women (CSW) (2020 – present)
- American Association of University Women (AAUW) at UAB (2019 – 2020)
- Faculty representative on UAB HPC Users Advisory Group (2016 - present)
- Graduate Students Thesis Committees at UAB (2006 – present)
- Faculty Advisor for Master and PhD students (2006 – present)
- Faculty Mentor, UAB Science and Technology Honor Program (2006 - present)
- Faculty Mentor, UAB Honors College (2006 - present)
- Faculty Mentor, UAB CORD summer research internship for high school students (2008 - present)
- Faculty Interviewer of the candidates for other graduate programs (2007 - present)
  - Medical Scientist Training Program
  - Graduate Biomedical Sciences

- Faculty Mentor, NSF REU program, Department of Physics (Summer 2011, 2012, 2014, 2015)
- Faculty Mentor, UAB's Beckman Scholars Program application for undergraduate research (2014)
- Faculty Judge for UAB BME Research Symposium (Spring 2012)
- Faculty Judge for graduate research day (Spring 2011)
- Associate Director of the Center for Computational and Structural Dynamics, UAB (2011 - 2012)
- Organizer of Molecular and Modeling Simulations study group monthly meetings (2011 - 2014)
- Advisory Board for mentoring women in computing and technology (2010 - 2012)
- Computer and Networking Advisory Committee, School of Engineering (2007 - 2009)
- Participation in UAB ADVANCE program (2006 - 2010)

### **Outreach Activities and Mentoring Female and Minority Students**

- Actively involved with the activities in Community OutReach Development program at UAB, mentoring minority high school students (2008 - present)
- School's representative on the UAB commission on the Status of Women (2020 – current )
- Faculty advisor for minority Undergraduate, Master and PhD students (2007 – present)
- Faculty advisor for female High School, Undergraduate, Master and PhD students (2007 – present)
- Faculty member for Society of Women Engineers, School of Engineering (2016 - present)
- Faculty Advisor for Society of Women Engineers, School of Engineering ( 2011 - 2016)
- American Association of University Women at UAB (2019)
- Faculty mentor for High school student in Hoover High School (2016-2017)
- Faculty mentor for High school student in Jefferson County International Baccalaureate School (2014-2015)
- Faculty mentor for High school students in Mountain Brook High School and Birmingham's Ramsay High School (2009)
- Advisory Board of mentoring for women in computing and technology, UAB (2010 - 2012)
- Committee for Professional Opportunities for Women, Biophysical Society ( 2012 - 2015)
- Early Careers Committee, Biophysical Society ( 2015 – 2017)
- Outreach with Girls, Inc. and Southern Company to highlight the fun in engineering through the Eureka!Nights program at Crestwood Center (2011)
- Outreach with Birmingham SWE Section and Southern Company to organize a Professional development series at UAB (2011, 2012)

### **Professional Service**

#### ***Grant reviews***

NSF CBET EBMS program, October 2021

UAB Center for Clinical and Translational Science (CCTS), November 2018

NSF CBET EBMS program, September 2018

NIH Membrane Biology and Protein Processing Study Section, October 2017

NSF CBET/CDS&E program, June 2017

Kentucky Science & Engineering Foundation, April 2016

Portuguese Foundation for Science and Technology, Panel Member for the Bioengineering, Biotechnology and Biochemistry Panel, Lisbon, Portugal, October 2012

#### ***Editorial Boards***

MCB: Molecular & Cellular Biomechanics (2007 - present)

Journal of Bioprocessing & Biotechniques (2011 - present)

Journal of Thermodynamics & Catalysis (2011 - present)

Health and Medical Informatics Open Access (2018 – present)

International Journal of Biochemistry & Physiology (2018 – present)

Membranes, Topic Editor in Section "Membranes in Life Science" (2021 – present)

#### ***Manuscript Reviews***

Computational and Structural Biotechnology Journal    Computational Biology and Chemistry

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Journal of Chemical Information and Modeling  
Biophysical Journal  
Journal of Biological Chemistry  
ACS Nano  
IEEE Transactions on Biomedical Engineering  
Journal of Mechanics in Medicine and Biology  
International Journal of Computational Bioscience  
Journal of Neurophysiology (panel review)  
The Journal of Arthroscopic and Related Surgery (panel review)

Medicinal Research Reviews  
Journal of Biomechanics  
Journal of Orthopedic Research (panel review)  
Clinical Biomechanics (panel review)

Biomechanics and Modeling in Mechanobiology  
PLoS ONE  
Computational Science & Discovery  
Materials & Design  
Journal of Zhejiang University-SCIENCE B  
Polymer Engineering and Science

### **Conference Organization**

Organizing committee for the 2013 Frontiers in Structure Biology of Membrane Proteins symposium

### **Research Support**

#### Ongoing Research Support

**NIH R01AG068395** (Role: PI) 09/15/2021 – 05/31/2026  
TREM2-endogenous ligand interactions in Alzheimer disease \$2,136,242 (TC)

**NSF/MCB MCB2024964** (Zhang, PI; role: collaborator) 08/01/2020 – 07/31/2024  
\$900,000 (TC)  
Regulatory functions of intrinsically disordered electronegative clusters (ENC) in RNA-binding proteins

**Alzheimer's Drug Discovery Foundation** (Roberson, PI; role: co-Investigator)  
04/01/2019 - 04/01/2023  
Toward Therapeutic Approaches to TREM2 in Alzheimer's Disease \$660,000 (TC)

**UAB Hugh Kaul Precision Medicine Institute pilot grant** (Role: PI) 05/01/2020 – 06/30/2023  
\$20,000 (TC)  
Repurposing already-available drugs to target human host proteins and SARS-CoV-2 proteins for COVID-19 prevention and treatment

#### Pending for Council Review

**NIH R01 AG081228-01** (Role: PI) 4/1/2023 - 03/31/2028  
Drugs repositioning to target TREM2 in Alzheimer's disease \$3,009,352 (TC)  
(Pending Council Review.  
Impact score: 33. FY 2022 pay line score: 40; FY 2023 pay line score: unknown)

#### Proposal to be Submitted in 11/14/2022

NIH R01 In response to Research on Current Topics in Alzheimer's Disease and Its Related Dementias (R01 Clinical Trial Optional) (PAR-22-093)

Molecular and structural bases of ApoE variants and TREM2-ApoE interactions in Alzheimer Disease (Role: PI)

#### Completed Research Support

**COVID-19 HPC Consortium spearheaded by White House of Science and Technology Policy, U.S. Department of Energy, NSF and IBM (TG-BIO200084)** (Role: PI) 12/03/2020 – 12/03/2021  
1,500,000 HPC service units (SUs)  
Computational Investigation of Vitamin D3 and its Hydroxyderivatives as Promising Drugs against COVID-19

**NIH R01 HL138990** (Qin, PI; role: co-Investigator) 07/1/2017 - 03/31/2021 \$375,000 (ADC)  
E2F2 and Vascular Function

**TG-BIO200050** (Role: PI) 01/01/2021 – 06/30/2021 100,000.0 SUs  
NSF-supported XSEDE Resource Allocations Committee (XRAC)

Integrative computational investigation of already-available drugs to target key human host and SARS-CoV-2 proteins for COVID19 treatment

**TG-MCB200181** (Role: PI) 06/17/2020 – 06/16/2021 50,000.0 SUs  
NSF-supported Extreme Science and Engineering Discovery Environment (XSEDE)  
Effects of Self-Oligomerization on Conformation and Ligand Binding in the Alzheimer's Disease Associated Protein TREM2

**NSF CBET-1159859** (Role: PI) 10/1/2012 - 09/30/2018 \$299,997 (TC)  
Thrombospondin-1/calreticulin binding in regulating cell intermediate adhesion and collagen expression

**Bioengineering-Surgery Collaborative pilot grant** (Role: MPI; Song and Parker) \$2500  
4/01/2017 – 03/31/2018

Synergistic Effect of Tamoxifen and TRA-8 on ER-Positive Breast Cancer Treatment

**AHA 14GRNT2048002** (Bevensee, PI; role: co-Investigator) 07/01/2014 – 06/30/2017 \$247,500 (TC)  
AHA (Southeast Affiliate) Molecular Physiology of Na/Bicarbonate Cotransporters

**NIH 5K25 CA140791** (Role: PI) 08/14/2009 – 06/30/2015 \$768,940 (TC)  
NIH/NCI Protein Interactions Underlying Fas-Mediated DISC in Cholangiocarcinoma

**NIH R01GM038953** (Falany, PI; role: co-Investigator) 9/30/2010 - 8/31/2014 250,000 (ADC)  
NIH/NIGMS Human Cytosolic Sulfotransferases

**TG-MCB130026** and **MCB130041** (Role: PI) 11/09/2012 – 11/08/2013 775,000 SUs  
NSF supported Extreme Science and Engineering Discovery Environment (XSEDE)  
The Interaction of PEG-grafted PLL Copolymers with Biomembrane

**Pilot award from UAB Center for Biophysical Sciences and Engineering** (Song, PI) \$2,500  
10/01/2011 - 09/30/2012

Characterize and quantify the studied protein-protein and protein-ligand interactions

**NSF TG-MCB090009** (Song, PI) 10/01/2008 - 09/30/2009

NSF's Partnerships for Advanced Computational Infrastructure

The role of thrombospondin 1-calreticulin interactions in calreticulin-induced intermediate adhesion

**NSF TG-MCB080078** (Song, PI) 04/21/2008 - 03/31/2009

NSF's Partnerships for Advanced Computational Infrastructure

In silico study of glycosylation effects on integrin structure and function

**UAB ADVANCE Faculty Research Awards through the sponsorship of NSF** (Song, PI) \$22,500  
07/01/2007 - 12/30/2008

Protein interactions underlying Fas-mediated apoptosis in osteoclasts

**NSF TG-MCB060053** (Baker, PI; Song, Co-PI) 07/01/2006 - 06/30/2007

Awarded as computational resources

NSF's Partnerships for Advanced Computational Infrastructure

Small molecule perturbation of biological membrane electrostatics, mechanics, and dynamics

## PUBLICATIONS

*With my students and co-advised students' names underlined; \* Corresponding author*

<http://www.ncbi.nlm.nih.gov/sites/myncbi/yuhua.song.1/bibliography/40758995/public/?sort=date&direction=descending>

Peer-reviewed Journal Articles (in reverse chronological order)

1. Andrzej T. Slominski, Tae-Kang Kim, Radomir M. Slominski, Yuwei Song, Zorica Janjetovic, Ewa Podgorska, Sivani B. Reddy, **Yuhua Song**, Chander Raman, Edith Kang, Adrian Fabisiak, Pawel Brzeminski, Rafal R. Sicinski, Venkatram Atigadda, Anton M. Jetten, Michael F. Holick, Robert C. Tuckey. Metabolic activation of tachysterol<sub>3</sub> to biologically active hydroxyderivatives in the human system that act on VDR, AhR, LXRs and PPAR $\gamma$  receptors. *The FASEB Journal*. 2022; 36(8): e22451. doi: <https://doi.org/10.1096/fj.202200578R>. (Impact Factor: 5.834)



2. Yuwei Song, Radomir M. Slominski, Shariq Qayyum, Tae-Kang Kim, Zorica Janjetovic, Chander Raman, Robert C. Tuckey, **Yuhua Song\***, Andrzej T. Slominski\*. Molecular and structural basis of interactions of vitamin D3 hydroxyderivatives with aryl hydrocarbon receptor (AhR): an integrated experimental and computational study. *International Journal of Biological Macromolecules*, 2022; 209:1111-23. doi: <https://doi.org/10.1016/j.ijbiomac.2022.04.048> PMID: 35421413 (Impact Factor: 6.953)
3. Brzeminski, Pawel; Fabisiak, Adrian; Slominski, Radomir; Kim, Tae-Kang; Janjetovic, Zorica; Podgorska, Ewa; Song, Yuwei; Saleem, Mohammad; Reddy, Sivani; Qayyum, Shariq; **Song, Yuhua**; Tuckey, Robert C. ; Atigadda, Venkatram; Jetten, Anton; Sicinski, Rafal; Raman, Chander; Slominski, Andrzej. Chemical synthesis, biological activities and action on nuclear receptors of 20S(OH)D3, 20S,25(OH)2D3, 20S,23S(OH)2D3 and 20S,23R(OH)2D3. *Bioorganic Chemistry*. 2022;121:105660. doi: <https://doi.org/10.1016/j.bioorg.2022.105660>. PMID: 35168121 PMCID: PMC8923993 (Impact Factor: 5.04)
4. Yuwei Song, Shariq Qayyum, Rory A Greer, Radomir M Slominski, Chander Raman, Andrzej T Slominski\*, **Yuhua Song\***. Vitamin D3 and its Hydroxyderivatives as Promising Drugs to Disrupt SARS-CoV-2 Entry against COVID-19: A Computational Study. *Journal of Biomolecular Structure and Dynamics*, 2021:1-17. Epub 2021/08/21. doi: 10.1080/07391102.2021.1964601. PubMed PMID: 344152182021 (Impact Factor: 3.549)
5. Aijun Qiao, Junlan Zhou, Shiyue Xu, Wenxia Ma, Chan Boriboun, Teayoun Kim, Baolong Yan, Jianxin Deng, Liu Yang, Eric Zhang, **Yuhua Song**, Yongchao Ma, Stéphane Richard, Chunxiang Zhang, Hongyu Qiu, Kirk Habegger, Jianyi Zhang, Marc Montminy, Gangjian Qin. Sam68 promotes hepatic gluconeogenesis via CRTC2. *Nature Communications*. 2021;12(1):3340. doi: 10.1038/s41467-021-23624-9. PMID: 34099657 PMCID: PMC8185084 (Impact Factor: 12.1)
6. Andrzej T Slominski\*, Tae-Kang Kim, Shariq Qayyum, Yuwei Song, Zorica Janjetovic, Allen SW Oak, Radomir M Slominski, Chander Raman, Joanna Stefan, Venkatram Atigadda, David K Crossman, Yaroslav Bilokin, Robert C Tuckey, Anton Jetten, **Yuhua Song\***. Biologically Active Vitamin D and Lumisterol Derivatives Act on Liver X Receptors (LXRs). *Scientific Reports*. 2021; 11: 8002, doi:10.1038/s41598-021-87061-w. PMID: 33850196 PMCID: PMC8044163 (Impact Factor: 4.120)
7. Yiming Zhang, Rory A Greer, Yuwei Song, Prithik Praveen, and **Yuhua Song\***. In silico identification of available drugs targeting cell surface BiP to disrupt SARS-CoV-2 binding and replication: Drug repurposing approach. *European Journal of Pharmaceutical Sciences*. 2021; 160:105771. PMID: 33617948 PMCID: PMC7894100 PMID: 33617948 <https://doi.org/10.1016/j.ejps.2021.105771> (Impact Factor: 3.616)
8. Daniel L. Kober, Melissa Brereton, Colin E. Kluender, Hunter B. Dean, Deborah F. Steinberg, Samantha Nelson, Berevan Baban, Carl Frieden, Jennifer Alexander-Brett, Erik D. Roberson, **Yuhua Song**, and Tom J. Brett. Functional insights from biophysical study of TREM2 interactions with ApoE and A $\beta_{1-42}$ . *Alzheimer's & Dementia. Featured Article*, 2021;17(3):475-88. PMID: 33090700 PMCID: PMC8026773 <https://doi.org/10.1002/alz.12194> (Impact Factor: 21.566)
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- analysis with experimental validation. *J Biomech.* 2004, 37(3):383-390. PMID: PMC1304055 (Impact Factor: 3.252)
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  52. Kaifeng Zhang, **Yuhua Song**. Analysis of thickness distribution control process of vacuum forming part by rigid visco-plastic shell FEM. *Journal of Plasticity Engineering*, 1997, 4(3):38-42

#### Invited Talks and Peer-reviewed Abstracts for Conference Presentation

1. Rory A Greer, Ryan A. Tuckey, Hunter B Dean, Erik D Roberson, **Yuhua Song**. Molecular and structural insight into the differences among common and rare Alzheimer's Disease-associated APOE variants. (under review) *67<sup>th</sup> Biophysical Society Annual Meeting*, Feb 18-22, 2023
2. Hunter B Dean, Rory A Greer, Jessica A Greven, Gunnar N Eastep, Daniel S Elston, Thomas J Brett, **Yuhua Song**, Erik D Roberson. Identification of novel small-molecule, endogenous ligands of the AD-associated microglial receptor TREM2 that increase its affinity for ApoE and induce cytoprotective immune activation. *Society for Neuroscience meeting 2022*. November 12-16, 2022 (To be presented)
3. Rory A Greer, Hunter B Dean, Thomas J Brett, Erik D Roberson, **Yuhua Song**. Identification of Endogenous Ligands for TREM2 through Unbiased Virtual Screening, *Biomedical Engineering Society Annual Meeting*, Oct 12-15, 2022
4. Hunter B Dean, Rory A Greer, Erik D Roberson, Thomas J Brett, **Yuhua Song**. AD-Associated TREM2 Variants Directly Impair Surface Interactions between the Hydrophobic Site of TREM2 and the Hinge Region of ApoE. Alzheimer's Association International Conference, July 31 – August 4, 2022

5. Andrzej T. Slominski, Tae-Kang Kim, Radomir M. Slominski, Yuwei Song, Zorica Janjetovic, Ewa Podgorska, Sivani B. Reddy, **Yuhua Song**, Chander Raman, Edith Kang, Adrian Fabisiak, Pawel Brzeminski, Rafal R. Sicinski, Venkatram Atigadda, Anton M. Jetten, Michael F. Holick, Robert C. Tuckey. Metabolic activation of tachysterol3 to biologically active hydroxyderivatives in the human system that act on VDR, AhR, LXRs and PPAR $\gamma$  receptors. *2022 Endocrine Society Annual Meeting*, June 11-14, 2022
6. Hunter B. Dean, Yuwei Song, Erik D. Roberson, **Yuhua Song**. Effects of Self-Multimerization on Conformation and Ligand Binding in the Alzheimer's Disease Associated Protein TREM2. *2022 Keystone Symposium - Neuro-Immune Interactions in the Central Nervous System*, June 5-9, 2022
7. Rory Greer, Gangjian Qin, **Yuhua Song**. Effect of Sam68 key residue mutations on its conformation and structure that may affect Sam68-mediated ECE-1b transcription. *66<sup>th</sup> Biophysical Society Annual Meeting*, Feb 19-23, 2022
8. Andrzej T Slominski\*, Tae-Kang Kim, Shariq Qayyum, Yuwei Song, Zorica Janjetovic, Allen SW Oak, Radomir M Slominski, Chander Raman, Joanna Stefan, Carlos A Mier-Aguilar, Venkatram Atigadda, David K Crossman, Andriy Golub, Yaroslav Bilokin, Edith K Y Tang, Robert C Tuckey, Anton M Jetten, **Yuhua Song**\*. Vitamin D and lumisterol hydroxyderivatives can act on liver X receptors (LXRs). *2021 Endocrine Society Virtual Annual Meeting*, March 20-23, 2021
9. Andrzej T. Slominski, Tae-Kang Kim, Shariq Qayyum, Radomir M. Slominski, Yuwei Song, Zorica Janjetovic, Ewa Podgorska, Edith K. Y. Tang, Yaroslav Bilokin, **Yuhua Song**, Chander Raman, Robert C. Tuckey, Michael F. Holick. Enzymatically-derived hydroxy-lumisterols regulate epidermal keratinocytes and act as agonists on aryl hydrocarbon receptor (AhR). *2021 Society for Investigative Dermatology (SID) Virtual Annual Meeting*, May 3-8, 2021
10. Andrzej T. Slominski, Tae-Kang Kim, Radomir M. Slominski, Shariq Qayyum, Yuwei Song, Zorica Janjetovic, Ewa Podgorska, Sivani Reddy, **Yuhua Song**, Chander Raman, Robert C. Tuckey, Venkatram Atigadda, Michael F. Holic. 20-hydroxytachysterol: synthesis and biological activity. *2021 Society for Investigative Dermatology Virtual Annual Meeting*, May 3-8, 2021
11. Rory Greer, Yuwei Song, Michael J. Patton, Matthew Might, Kevin S. Harrod, Chad M. Petit, **Yuhua Song**\*. Identification of FDA approved antiviral drugs for COVID-19 treatment using unbiased virtual screening. *65<sup>th</sup> Biophysical Society Annual Meeting*, Feb 22-26, 2021
12. Yuwei Song, Shariq Qayyum, Radomir M Slominski, Chander Raman, Andrzej T Slominski\*, **Yuhua Song**\*. Vitamin D and its Derivatives as Promising Drugs against COVID-19 - A Computational Study. *65<sup>th</sup> Biophysical Society Annual Meeting*, Feb 22-26, 2021
13. Hunter Dean, Thomas Brett, Erik Roberson\*, **Yuhua Song**\*. Developing a Functionally Valid Model of the TREM2-ApoE Complex to Better Understand its Role in Alzheimer's Disease. *65<sup>th</sup> Biophysical Society Annual Meeting*, Feb 22-26, 2021
14. Yiming Zhang, Yuwei Song, Hrithik Praveen, **Yuhua Song**\*. *In Silico* Identification of Drugs that Could Neutralize SARS-CoV-2 Binding and Falter Viral Replication through Cell Surface BiP. *BMES 2020 Virtual Annual Meeting*, October 14-17, 2020
15. Shariq Qayyum, Tae-Kang Kim, Radomir M. Slominski, Zorica Janjetovic, Yuwei Song, Allen C. Oak, Hanumanthu V. Sagar, Raman Chandar, Purushotham Guroji, Yaroslav Bilokin, **Yuhua Song**, Anton Jetten, Robert C. Tuckey and Andrzej T. Slominski. CYP11A1-derived hydroxy-lumisterols act as agonists on LXR $\alpha$  and  $\beta$ . Presented in 2020 Society for Investigative Dermatology (SID) Virtual Annual Meeting, May 13-16, 2020
16. Dean HB, Roberson ED, **Song Y**\*. Frontotemporal Dementia–Associated Variants Destabilize the Apical Ligand-Binding Region of the TREM2 Immunoglobulin Domain. *BMES 2019 Annual Meeting*, October 16-19, 2019; Philadelphia, PA
17. Romone Fancy, Tiara S. Napier, Qinghua Zeng, Donald J. Buchsbaum, Catherine C. Parker, **Yuhua Song**\*. Potential mechanism for synergistic cytotoxicity of TRA-8 and tamoxifen in ER-positive MCF-7 breast cancer cells. *BMES 2018 Annual Meeting*, October 17-20, 2018; Atlanta, GA
18. Dean HB, Roberson ED, **Song Y**\*. The Effects of Common Disease-Causing Variations on the Structure and Stability of TREM2: An *In Silico* Examination. 1st Annual Southeastern Neurodegenerative Disease Conference; 2018 Sept 27-29; Orlando, FL.

19. **Yuhua Song**. Integrated computational and experimental study of death receptor-mediated apoptotic signaling in breast cancer. *Shandong University-Qingdao campus, Qingdao, China, July, 2018* (Invited Talk).
20. Romone M. Fancy, Jun Li, Huixian Hong, John D. Mountz, Joanne E. Murphy-Ullrich, Santosh K. Katiyar, Jianyi Zhang, **Yuhua Song**<sup>\*</sup>. Cell surface calreticulin-LRP1 binding and its role in apoptotic cell engulfment. *Biophysical Society 62th Annual meeting*, Feb 17-21, 2018, San Francisco, CA.
21. Lingyun Wang, Joanne Murphy-Ullrich, Jianyi Zhang, **Yuhua Song**<sup>\*</sup>. Multiscale Modeling of Dynamic Interactions between Calreticulin and a Model Membrane Microdomain. *BMES 2017 Annual Meeting*, October 11-14, 2017, Phoenix, AZ.
22. Hongyi Yang, Joanne E. Murphy-Ullrich, **Yuhua Song**<sup>\*</sup>. Molecular Insights for the Role of Key Residues of Calreticulin in its Binding Activities. *Biophysical Society 60th Annual meeting*, 2016.
23. **Yuhua Song**, Protein interactions underlying death receptor 5-mediated death inducing signaling complex in apoptosis, UAB Research Computing Day, September, 2016 (Invited Talk).
24. Romone Fancy, Donald J. Buchsbaum, Tong Zhou, **Yuhua Song**<sup>\*</sup>. Calmodulin-DR5 binding in breast cancer: Independent of TRA-8 sensitivity. [abstract]. In: *Proceedings of the 106th Annual Meeting of the American Association for Cancer Research*; 2015 Apr 18-22; Philadelphia, PA. Philadelphia (PA): AACR; *Cancer Res* 2015;75 (15 Suppl):Abstract nr 2931. doi:10.1158/1538-7445.AM2015-2931
25. Lingyun Wang, Joanne E. Murphy-Ullrich, **Yuhua Song**<sup>\*</sup>. Effect of an apoptotic membrane raft on the conformational and dynamical changes of calreticulin. *Biophysical Society 59th Annual meeting*, February, 2015.
26. Romone Fancy, Hong Wang, Tong Zhou, **Yuhua Song**<sup>\*</sup>. Calmodulin binding to DR-5 and the role of CaM-DR-5 binding in DR-5-mediated DISC formation in breast cancer. [abstract]. In: *Proceedings of the 105th Annual Meeting of the American Association for Cancer Research*; 2014 Apr 5-9; San Diego, CA. Philadelphia (PA): AACR; *Cancer Res* 2014;74 (19 Suppl):Abstract nr 2282. doi:10.1158/1538-7445.AM2014-2282
27. Lingyun Wang, Joanne E. Murphy-Ullrich, **Yuhua Song**<sup>\*</sup>. Molecular insight for the effect of lipid raft on thrombospondin-1 and calreticulin interactions. *Biophysical Society 58th Annual meeting*, February, 2014
28. **Yuhua Song**. Protein interactions underlying death receptor-mediated death inducing signaling complex in apoptosis. *International Conference on Oncology and Therapy, Beijing, July, 2013* (Invited Talk).
29. **Yuhua Song**. The Role of Thrombospondin-1 Binding to Calreticulin in Focal Adhesion Disassembly – A Computational Study. *International Conference on Biomedical Engineering, Beijing, June, 2013* (Invited Talk).
30. Tiara Napier, Romone Fancy, Tong Zhou, John Mountz, **Yuhua Song**<sup>\*</sup>. Effect of the combined treatment of TRA-8, an agonistic DR5 antibody, and tamoxifen on breast cancer cells. [abstract]. In: *Proceedings of the 104th Annual Meeting of the American Association for Cancer Research*; 2013 Apr 6-10; Washington, DC. Philadelphia (PA): AACR; *Cancer Res* 2013;73 (8 Suppl):Abstract nr 2955. doi:10.1158/1538-7445.AM2013-2955.
31. Lingyun Wang, **Yuhua Song**<sup>\*</sup>. Structural and dynamical changes for different types of lipid bilayer by different length of poly-L-lysine: MD simulations. *Biophysical Society 57th Annual meeting*, February, 2013
32. Romone Fancy, Tiara Napier, Lingyun Wang, Gu Jing, Jay M McDonald, Tong Zhou, **Yuhua Song**<sup>\*</sup>. Characterize calmodulin/Fas death domain interaction with combined ITC, CD and computational studies. *BMES 2012 Annual Meeting*, October 2012.
33. Romone Fancy, Tiara Napier, Gu Jing, Jay M McDonald, Tong Zhou, **Yuhua Song**<sup>\*</sup>. Quantitative characterization of calmodulin and Fas death domain interactions. [abstract]. In: *Proceedings of the 103rd Annual Meeting of the American Association for Cancer Research*; 2012 Mar 31-Apr 4; Chicago, IL. Philadelphia (PA): AACR; *Cancer Res* 2012;72(8 Suppl):Abstract nr 4754. doi:1538-7445.AM2012-4754

34. Lingyun Wang, Di Pan, Qi Yan, Russell Green, **Yuhua Song\***. Activation mechanisms of  $\alpha V\beta 3$  integrin by binding to fibronectin: a computational study. *Biophysical Society 56th Annual meeting*, February 2012.
35. Qi Yan, Jay M McDonald, **Yuhua Song\***. Structural insight for the role of Fas binding to FADD and oligomerization degree of Fas/FADD complex in death inducing signaling complex formation. [abstract]. In: *Proceedings of the 102nd Annual Meeting of the American Association for Cancer Research*; 2011 Apr 2-6; Orlando, FL. Philadelphia (PA): AACR; *Cancer Res* 2011;71(8 Suppl):Abstract nr 19. doi:10.1158/1538-7445.AM2011-19.
36. Qi Yan, Joanne E, Murphy-Ullrich, **Yuhua Song\***. Molecular and structural insight for the role of key residues of thrombospondin-1 and calreticulin in thrombospondin-1- calreticulin binding. *Biophysical Society 55th Annual meeting*, March 2011.
37. Di Pan, Qi Yan, Yabing Chen, Jay M McDonald, **Yuhua Song\***. Conformational and thermodynamics analyses of the regulation of trifluoperazine in camodulin binding to Fas: Implications for cancer chemotherapy. [abstract]. In: *Proceedings of the 101st Annual Meeting of the American Association for Cancer Research*; 2010 Apr 17-21; Washington, DC. Philadelphia (PA): AACR; *Cancer Res* 2010;70 (8 Suppl):Abstract nr 96.
38. Di Pan, **Yuhua Song\***. Effect of the conjugation of PEG to the PLL on the micro- and mesoscopic properties of a POPC bilayer. *Biophysical Society 54th Annual meeting*, February 2010.
39. Qi Yan, Joanne E, Murphy-Ullrich, **Yuhua Song\***. Modeling of the structural basis of thrombospondin-1 and calreticulin interactions. *Biophysical Society 53th Annual meeting*, March 2009.
40. Di Pan, Qi Yan, **Yuhua Song\***. Effect of Trifluoperazine on  $Ca^{2+}$ -Bound Calmodulin binding to Fas Death Domain for DISC Formation. *Biophysical Society 53th Annual meeting*, March 2009.
41. Jonathan Suever, Yabing Chen, Jay M. McDonald, **Yuhua Song\***. Conformation and Free Energy Analyses of the Complex of  $Ca^{2+}$ -Bound Calmodulin and the Fas Death Domain. Southeastern Meeting of the American Society for Biomechanics, April 2008.
42. Di Pan, **Yuhua Song\***. Effect of Altered Glycosylation on Binding Affinity of Beta1 I-Like Domain with Fibronectin. Southeastern Meeting of the American Society for Biomechanics, April 2008.
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