

Yayin Fang, Ph.D.

Professor

Contact Information

Department of Biochemistry & Molecular Biology

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Education

Ph.D. in Physical Chemistry, Nankai University, Tianjin, China, 2001

Teaching

- First Year Medical Course: Molecules and Cells Unit IB
- Dental Biochemistry
- General Biochemistry
- General Biochemistry Laboratory
- Protein Structure and Function
- Orientation to Research

Research Interests

Molecular modeling and MD simulation on DNA recognition

Structure based and ligand-based drug design

Polymeric material design

Grants and Awards

- **NIH/NIDCR** (R25DE032527) 12/01/2022 - 11/30/2027, Role: Co-PI.
- **NSF** (1924092) 10/01/2019 - 09/31/2022, Role: Co - PI.
- **NSF** (1708959) 9/01/2017 - 8/31/2022, Role: PI.
- **NIH/NIMHD** (2U54MD007597) 06/01/2019 –01/31/2024. Role: Co-I.
- **The Office of Naval Research**(N00014-19-1-2602). PI: Yayin Fang. 08/01/2019 - 7/31/2021. Role: PI.
- **The Office of Naval Research**(N00014-18-1-2145). 03/01/2018 - 2/28/2020.

- Role: PI.
- **The Office of Naval Research**(N00014-17-1-2105). 03/01/2017 - 08/31/2018. Role: PI.
 - **NSF-The Howard University HU ADVANCE-IT Mini Grant**. 05/01/2016 – 04/30/2017. Role: PI.
 - **NSF-The Howard University HU ADVANCE-IT Mini Grant**. 10/01/2014 – 09/30/2015. Role: PI.
 - **The Howard University Bridge Funds and Pilot Study Awards Program (BFPSAP)**. 11/01/2012 – 10/31/2013. Role: PI.
 - **HUMAA (Howard University Medicine Alumni Association) Endowed Founder’s Chair in Basic Science**, Howard University, College of Medicine, July 2015.
 - **HU ADVANCE-IT Achievement Award**. Howard University, May 4, 2015.
 - **AACR Minority-Serving Institution Faculty Scholar in Cancer Research Award** to attend the upcoming AACR Special Conference on *Computational Systems Biology of Cancer* being held on February 9 – 11, 2015, the Fairmont, San Francisco, CA.
 - **Most outstanding Presentation by a Junior Faculty Researcher of Computation & Modeling** at the 2014 Howard University Research Day on April 4, 2014.
 - **Excellent Presentation Award** by the American Chemical Society-Indiana Section at the 4th Annual ACS Poster Session on Oct. 8, 2003.

Selected Publications

1. Nida Ali Alsaffar, **Yayin Fang**, Eric Walters. “Thymoquinone Effect on the Dictyostelium discoideum Model Implicates Functional Roles for Glutathione S-transferases in Eukaryotic Proliferation, Chemotaxis, and Development.” *PLOS ONE*, 3/1/2023. <https://doi.org/10.1371/journal.pone.0282399>
2. Jessica L. Fletcher, Grant Mahant, Tyler J. Witzleb, Riley Busche, **Yayin Fang**, Eugene J. Billiot, Fereshteh H. Billiot, Kevin F. Morris. “NMR Investigation of Counterion Binding to Undecyl LL-Leucinevalanate Micelles.” *Journal of Dispersion Science and Technology*, 12/13/2022. <https://doi.org/10.1080/01932691.2022.2145303>
3. Patrice Moss, Galina Talanova, **Yayin Fang**, Courtney Thomas. “Spectroscopic studies of 7,8-diacetoxy-4-methylcoumarin and 7,8-dipentynoyl-4-methylcoumarin binding with Calreticulin” *The Journal of Biological and Chemical Luminescence*, 2022,1,11. <https://doi.org/10.1002/bio.4362>
4. Raina Rhoades, Brianna Henry, Dominique Prichett, **Yayin Fang**, Shaolei Teng. “Computational Saturation Mutagenesis to Investigate the Effects of Neurexin-1 Mutations on AlphaFold Structure” *Genes*, 2022, 13, 789.
5. Kevin F. Morris, Riley Geoghegan, Emily Palmer, Matthew George, Jr. and **Yayin Fang***. "Molecular Dynamics Simulation Study of AG10 and Tafamidis Binding to the Val122Ile Transthyretin Variant." *Biochemistry and Biophysics Reports*, 2020, 21, 100721.
6. Kevin F. Morris, Eugene J. Billiot, Fereshteh H. Billiot, Jordan A. Ingle, Kevin B. Krauss, Corbin R. Lewis, Kenny B. Lipkowitz, William M. Southerland, and **Yayin Fang***. “Using

- Molecular Dynamics Simulations to Identify the Key Factors Responsible for Chiral Recognition by an Amino Acid-based Molecular Micelle.” *Journal of Dispersion Science and Technology*, 2019, 40(5), 716-727.
- Kevin F. Morris, Eugene J. Billiot, Fereshteh H. Billiot, Jordan A. Ingle, Stephanie R. Zack, Kevin B. Krauss, Kenny B. Lipkowitz, William M. Southerland, and **Yayin Fang***. “Investigation of Chiral Recognition by Molecular Micelles with Molecular Dynamics Simulations.” *Journal of Dispersion Science and Technology*, 2018, 39(1), 45-54.
 - Linyong Mao, **Yayin Fang**, Michael Campbell, and William M. Southerland. “Population Differentiation in Allele Frequencies of Obesity-Associated SNPs.” *BMC medicinal Genomics*, 2017, 18 (1), 861-876.
 - Kevin F. Morris, Eugene J. Billiot, Fereshteh H. Billiot, Kenny B. Lipkowitz, William M. Southerland, **Yayin Fang***, "Molecular Dynamics Simulation and NMR Investigation of the Association of the β -Blockers Atenolol and Propranolol with a Chiral Molecular Micelle.", 2015, *Chemical Physics*, 457, 133-146.
 - Kevin F. Morris, Eugene J. Billiot, Fereshteh H. Billiot, Kenny B. Lipkowitz, William M. Southerland, **Yayin Fang***, "A Molecular Dynamics Simulation Study of the Association of 1,1'-Binaphthyl-2,2'-diyl hydrogen phosphate Enantiomers with a Chiral Molecular Micelle.", 2014, *Chemical Physics*, 439, 36-43
 - Kevin F. Morris, Eugene J. Billiot, Fereshteh H. Billiot, Kenny B. Lipkowitz, William M. Southerland, **Yayin Fang***, "A Molecular Dynamics Simulation Study of Two Dipeptide Based Molecular Micelles: Effect of Amino Acid Order ", 2013, *Open Journal of Physical Chemistry*, 3, 20-29
 - Kevin F. Morris, Eugene J. Billiot, Fereshteh H. Billiot, Kenny B. Lipkowitz, William M. Southerland, **Yayin Fang***, "Investigation of Chiral Molecular Micelles by NMR Spectroscopy and Molecular Dynamics Simulation", 2012, *Open Journal of Physical Chemistry*, 2, 240-251
 - Patrice L. Jackson, K.R. Scott, William M. Southerland, and **Yayin Fang***, “Enaminones 8: CoMFA and CoMSIA Studies on Some Anticonvulsant Enaminones”, *Bioorganic & Medicinal Chemistry*, 2009, 17, 133-140
 - Pedro R. Romero, Saima Zaidi, **Yayin Fang**, Vladimir N. Uversky, Predrag Radivojac, Christopher J. Oldfield, Marc S. Cortese, Megan Sickmeier, Tanguy LeGall, Zoran Obradovic and A. Keith Dunker, “Alternative Splicing in Concert with Protein Intrinsic Disorder Enables Increased Functional Diversity in Multicellular Organisms”, *Proceedings of the National Academy of Sciences of the United States of America*; 2006, 103(22), 8390-8395
 - Yayin Fang**; Kenny B. Lipkowitz and Eric C. Long, “Molecular Dynamics Simulations of the Orientation of Ni(II)•Gly-Gly-His and Ni(II) •Arg-Gly-His Metallopeptide-DNA Association”, *Journal of Chemical Theory and Calculation*, 2006, 2(5); 1453-1463
 - Yayin Fang**; Craig A. Claussen; Kenny B. Lipkowitz and Eric C. Long, "Diastereoselective DNA Cleavage Recognition by Ni(II)•Gly-Gly-His Derived Metallopeptides", *Journal of the American Chemical Society*, 2006, 128(2), 3198 – 3207
 - Yayin Fang**, Bruce D. Ray, Craig A. Claussen, Kenny B. Lipkowitz and Eric C. Long, "Ni(II)•Gly-Gly-His Derived Metallopeptide-DNA Interactions: Structural Characterization of Minor Groove Binding and Recognition", *Journal of the American Chemical Society*, 2004, 126(17), 5403 – 5412.

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