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RESEARCH INTERESTS & PERSONAL STATEMENT

- Molecular Evolution for emerging diseases (SARS-COV-2, Influenza A/H3N2, Monkeypox, Dengue, West Nile virus, Zika, Enterovirus D68, Mumps, Measles, West African Ebola, RSV-A/B and Tuberculosis)
- Activation of Immuno-Receptors (CAR-T and TLRs)
- Computer-aided Drug Designs (CADD) of small-molecule drugs and mRNA vaccines
- Bioinformatics tools, Molecular Modeling (MM) and Molecular Dynamics Simulation (MD)
- Administrator, Programmer and User of High Performance Computer (HPC)

Dr. Chun Wu is a tenured associate professor with a joint appointment in the Departments of Chemistry & Biochemistry and Biological Biomedical Sciences at Rowan University. He earned his PhD from the University of Delaware, where he worked on protein force field development and conducted molecular dynamics simulations of amyloidogenic peptides. He later pursued postdoctoral training at the University of California, Davis, and Santa Barbara, focusing on developing structural models of amyloidogenic peptide oligomers.

At Rowan University, Dr. Wu's lab is pioneering a bioinformatics tool—the substitution-to-mutation rate ratio (C/μ) test—to quantify the fitness effects of mutations directly from genomic sequence data. Applied to viral genomes, the method has given rise to the Near-Neutral Selectionist Theory (NNST), a novel framework that clarifies the molecular evolution of SARS-CoV-2 and other pathogens while pinpointing genomic hotspots vital for designing both current and next-generation vaccines and therapeutics to combat infectious diseases.

In his computer-aided drug design (CADD) lab, Dr. Wu's team employs molecular docking, homology modeling, and molecular dynamics simulations to investigate the binding interactions between protein receptors and ligands for novel drug discovery. Collaborating with experimental groups, the Wu lab strives to identify new protein receptors and small molecules with potential applications as anti-cancer, antiviral, and anti-neurodisorder agents, while also optimizing ionic liquids for the stabilization of proteins and nucleic acids.

With over 110 peer-reviewed publications, external research funding totaling $1.5 million, and 3.3 million CPU hours as a Principal Investigator (PI) and co-PI, he has achieved an h-index of 39 with more than 10,136 citations. His pioneering works in bioinformatics, computational biochemistry, molecular modeling, simulation, and computer-aided drug design (CADD) has earned him recognition from peers worldwide. He has been invited to present at numerous national and international conferences, including prestigious institutions in China. In 2021, he was named a World Class Professor by the Indonesia Ministry of Education and Culture, and his CADD lab received the Rowan University Breakthrough of the Year Award in 2023.

In addition to his research, Chun is deeply committed to teaching and mentoring students at both the undergraduate and graduate levels. During his time at the Computational Science Research Center (CSRC), he co-supervised two postdoctoral researchers—Uba and Vikash. Uba has since become an Assistant Professor in the Department of Molecular Biology and Genetics at Istanbul AREL University, Turkey, as of February 2023. At Rowan University, Chun has mentored over 34 Master's students and 120 undergraduates, contributing to 51 publications and 152 conference posters.

EDUCATION

2005	Ph. D.	Computational Biochemistry	**University of Delaware**, Newark, DE
2005	M. S.	Computer Science	**University of Delaware**, Newark, DE
1999	M. S.	Analytical Chemistry	**Xiamen University**, China
1995	B. S.	Chemistry	**Xiamen University**, China

PROFESSIONAL EXPERIENCE

2018-present	Associate Professor, **Rowan University, Depts of Chemistry & Biochemistry and Biological & Biomedical Sciences, Rowan University**, Glassboro, NJ 08028.
2018- 2023	Associate member of **Beijing Computational Science Research Center (CSRC)**
2018 - 2019	Bioinformatics Program Coordinator, **Dept. of Molecular & Cellular Biosciences, Rowan University**, Glassboro, NJ 08028.
2013 - 2018	Assistant Professor, **Depts of Chem & Biochemistry and Molecular & Cellular Biosciences, Rowan University**, Glassboro, NJ 08028.
2011 - 2013	Research Assistant Professor, Department of Chemistry and Biochemistry **University of California, Santa Barbara**, CA 93106
2009 - 2011	Assistant Specialist, Department of Chemistry and Biochemistry **University of California, Santa Barbara**, CA 93106
2007 - 2009	Postdoctoral Fellow, **Department of Chemistry and Biochemistry** **University of California, Santa Barbara**, CA 93106 Postdoctoral Research with Joan-Emma Shea. PhD and Michael T. Bowers, PhD, Dept of Chem and Biochemistry, UCSB
2005 - 2006	**University of California, Davis,** CA 95616 Postdoctoral Fellow, the Genome Center of UC Davis Postdoctoral Research with Yong Duan, PhD, UC Davis

EXTRAMURAL FUNDING

Normal grants (Total awarded external grants **$1.65 million** as PI and Co-PI)

2024-2027	Faculty Mentor, **C Wu**, NIH-T34, Bridges to the Baccalaureate
2024-2025	Lead PI: **C WU**, Co-PIs: XY Mou, Study of PI-111 as Topical Muscle Relaxant, New Jersey Commission on Science, Innovation and Technology **($40,000)**
2024-2025	Lead PI: **C WU**, Co-PIs: XY Mou**,** S. Jonnalagadda, *Joint Computational-Experimental Discovery of novel HAC6 inhibitors for treating triple-negative breast cancer (TNBC)* New Jersey Health Foundation (PC 76-23) **($50,000)**
2022-2025	Lead PI: Xiao-Yang Mou, Co-PIs: **C WU,** S. Jonnalagadda, M. Pandey, *Novel inhibitors of RNA-dependent RNA Polymerase (RdRp) of SARS-CoV-2 as effective COVID-19 therapeutics - An experimental and computational study*, Guava Medicine LLC, **($140,000)**
2021-2024	**C, WU** (Faculty Mentor), NIH, Undergraduate Research Training Initiative for Student Enhancement (U-RISE) training grant (T34)
2021-2023	Lead PI: **C Wu**, Co-PI, T Keck, *Joint Computational-Experimental Drug Discovery Of Novel Biased Agonists to Dopamine D2 Receptor toward Better Schizophrenia/Parkinson's Medications,* New Jersey Health Foundation **($35,000**)
2019-2022	Lead PI: **C WU**, Co-PI, Dr. Abdullahi Ibrahim Uba, Computer Aided Drug Design in targeting GPCRs and anti-cancer anti-body, Postdoc Fellowship (**$100,000)**, Beijing Computational Science Research Center, Beijing, 100193 P. R. China
2019-2021	Lead PI: **C WU**, Co-PI: Dr. Vikash Kumar, Computer Aided Drug Design in targeting GPCRs and anti-cancer anti-body, Postdoc Fellowship **($100,000**), Beijing Computational Science Research Center, Beijing, 100193 P. R. China
2019-2023	Lead PI: T Vaden Co-PIs: **C WU** and G Caputo, *RUI: Combining Experiments and Simulations To Optimize Biomolecular Ionic Liquids for Protein Stabilization,* NSF DMR-1904797 **($300,000**)
2018-2020	Lead/Host PI: **C WU**, Co-PI: Dr. Dr. Siyan Liao, Computer Aided Drug Design in targeting GPCRs and anti-cancer anti-body, Visiting scholarship (Guangzhou Medical University, Guangzhou, 511436 P. R. China, (**$100,000)**

2018-2019 Lead PI:C. Krummenacher Co-PI:**C WU** *Development of small inhibitors of herpes simplex virus (HSV) infection*. New Jersey Health Foundation **($ 35,000**)

2016-2017 Lead PI: Dimitri Pestov, Co-PI: **C WU**, *Targeting ribosome biogenesis as a new strategy to enhance cancer chemotherapy,* New Jersey Health Foundation, (**$ 35,000)**

2016-2017 Lead PI: Subash Jonnalagadda, Co-PI: **C WU**, *Development of Novel Small Molecules as Potential Anti-Cancer Agents,* Channel Therapeutics Industry award (**$62,479)**

2015-2017 Multi-PI: **C Wu** TM Keck, G Moura-Letts. Understanding the Consequences of 6TM Splice Variants in MOR-1 Ligand Binding: Towards Novel Analgesics, Channel Biosciences **($205,620 total**).

2014-2017 Lead PI: Nidhal Bouaynaya, Co-PIs: **C Wu**, Robi Polikar, and B. Sukumaran, "*MRI: Acquisition of a High Performance Computer to Integrate Data Intensive Research and Education: Bringing HPC to South Jersey*," The National Science Foundation (**ACI-1429467**) hereby awards a grant of (**$397,024)** to Rowan University for support of the project described in the proposal referenced above as modified by cover page dated February 25, 2014.

2015-2016 Host PI:**C WU**, Co-PI: Dr. Kai Tan *Development and application of QM/MM (Quantum Mechanics/Molecular Mechanics) methods to study Metalloproteins,* China Scholarship Council (**CSC-201406315045, $21,600**)

2015-2016 Host PI: **C Wu**, Co-PI: Dr. Dr. Xiaoyan Wang, *Drug design of Type 2 diabetes mellitus (T2DM) against targets β3-AR and GLP-1R by molecular dynamics simulation*, Visiting scholarship **$8,000** (Shandong Provincial Education Department)

Supercomputer Time grants

(Total awarded Supercomputer Time **3.3 million CPU hours** with equivalent value of $732,645 as PI)

2022-2024 Sole PI: **C WU**, *To probe the activation mechanism of HER2 directed Chimeric T-Cell Receptor (CAR) using molecular dynamics simulation with explicit membrane*, National Research Council at the National Academies of Science, **MCB170090P** (**460,000 MD** Simulation Units) on Anton2 at Pittsburgh Supercomputing Center. It was pressed in Rowan Today.

2017-2025 Sole PI: **C WU**, *Request of computational time for a bioinformatics course in Fall* National Science Foundation: **ACCESS/BIO230145 or MCB170088** (**7 x *200,000 SUs,***)

2020-2021 Sole PI: **C WU**, *In silico visioning communications between signal ligands bound to β2 adrenergic G-protein coupled receptor (GPCR) and effecter guanine nucleotide (GDP) bound to Gα in an open conformation using molecular dynamics simulations in explicit membrane*, National Research Council at the National Academies of Science, **MCB170090P** (**150,000 MD** Simulation Units) on Anton2 at Pittsburgh Supercomputing Center (PSC). Anton 2 is a second-generation special-purpose supercomputer for molecular dynamics simulations, which is 180 times faster than general-purpose supercomputer.

2017-2018 Sole PI: **C WU,** *Probe activation mechanism of membrane GPCR receptors using all-atom molecular dynamics simulation with explicit membrane*. National Research Council at the National Academies of Science, **PSCA17017P** (**100,000 MD** Simulation Units on Anton 2 at Pittsburgh Supercomputing Center (PSC)

2016-2018 Sole PI: **C WU**, *Request of computer time on Stampede for a modeling course in Spring 2017,* National Science Foundation **MCB160004** (**2** x ***200,000 SUs),*** Sole PI: **C WU**, *Request of computer time to study the activation mechanism of 6TM variants of human μ-opioid receptor by morphine derivative (IBNtxA) using all-atom molecular dynamics simulation with explicit membrane* Action Type: National Science Foundation, **MCB160164** (***200,000 SUs)***

2016-2017 Sole PI: **C. WU**, *Probe activation mechanism of membrane receptors using all-atom molecular dynamics simulation with explicit membrane,* National Science Foundation, **MCB160173** (**230,000 SUs**)**.**

INTRAMURAL FUNDING

2017-2018 Lead PI: **C Wu**, Co-PI, T Keck, *Joint Computational-Experimental Drug Discovery*

Of Novel Biased Agonists to Dopamine D2 Receptor toward Better Schizophrenia/Parkinson's Medications, College of Science and Mathematics (CSM) Pilot Seed Fund **($20,000**)

2015-2016 Sole PI**: C Wu**, *Binding of anticancer ligands (telomestatin and its novel replacement) to key G-Quadruplex DNA structures probed by molecular dynamics simulations,* Rowan University Seed Funding Program **($10,000**)

2013-2016 Sole PI: **C Wu**, Rowan startup **($80,000**)

PENDING RESEARCH PROPOSAL

2024-2025 Sole PI: **C WU**, Can Near-Neutral Balanced Selectionist Theory (NNBST), a Quantitative Evolution Theory, Explain Genomic Evolution of SARS-CoV-2 and Other Deadly Viruses? NSF (**$854,132**)

2025-2028 PI, T Vaden, Co-PIs: Caputo and **Wu**, Assessing the effects of amino acid - fatty acid ionic liquids on copper proteins, NSF **($566,022**)

2024-2028 PI: **C WU**, Co-PI: S. Jonnalagadda, Optimizing biased M3 mAChR small molecule ligand to mitigate airway pathology in asthma, Subcontractor under NIH R61/R33 TJU-Rowan Grant **($582,024)**

2023-2025 Multiple PIs: Krummenancher, C, S. Jonnalagadda, **C Wu,** Structure-based design of inhibitors of HSV entry, NIH R15, **$441,510**

2022-2025 Faculty Mentor, **C Wu**, NSF, REU Site: Research and Career Development in Pharmaceutical Chemistry, 2022-2025, **$350,000**, Pending

2025-2028 Senior Investigator, **C Wu**, NSF, MRI: Track 1 Acquisition of a High-Performance CPU/GPU/High-Memory Computing System to Empower Scientific Advancementand Innovation at Rowan University **$1,397,340** Pending

AWARD

1995 Excellent Graduation Paper, Department of Chemistry, Xiamen University
1999 Excellent Thesis, Department of Chemistry, Xiamen University
2004 Dean's list, University of Delaware
2009 Travel Award, Gordon research conference: Biol. Mol.in Gas Phase and in Solution
2021 The World Class Professor by Indonesia Ministry of Education and Culture, Republic of Indonesia
2023 the Rowan University Breakthrough of the Year Award

PEER REVIEWED PUBLICATIONS (109 total, h-index 37, total citations 10136+)

https://scholar.google.com/citations?user=vk54XEgAAAAJ&hl=en
http://www.researcherid.com/rid/J-2005-2012
http://orcid.org/0000-0002-0176-3873
https://www.ncbi.nlm.nih.gov/sciencv/

Peer Reviewed Publications since Joining Rowan Univ. (Undergrad Students Underlined)

2025:

1. Liao, S.; Pino, M. J.; Li, Y.; Wu, C. Identification of potential antagonists of Human TAAR1 for possible treatment of Parkinson's disease using structure-based virtual screening and molecular dynamics simulation. 2025, under review.

2. Abdullahi Ibrahim Uba, John Chea, Amber Elizabeth Mott, Jasmine Essence Mott, and **Chun Wu***, Effects of Taxol binding on the dynamic instability of tubulin dimer-GDP interface investigated using all-atom molecular dynamics simulation with explicit solvent, **Journal of Molecular Recognition,** 2025 under review

3. Mariya Hryb, Leah Davis, Stefi Lao, Nichole Daringer, Xiaoyang Mou and **Chun Wu***, To probe activation mechanism of HER2 directed Chimeric T-Cell Receptor (CAR) by antigen using homology modeling and all-atom molecular dynamics simulation, **Computational Biology and Medicine**, 2025 under review

4. Wu, C.; Paradis, N. Near Neutral Selectionist Theories for SARS-COV-2 suggested by substitution-mutation ratio (c/μ) test **2025**, Under preparation.

5. Chun Wu, Nicholas J. Paradis, Khushi Jain, Balanced Condition for Near Neutral Selectionist Theories and a guide on using substitution-mutation rate ratio (c/u) to decipher evolution. **Genome and Biology Evolution**, **2025**, Under review.

6. Wu, C.; Paradis, N. J.; Jain, K. Substitution-Mutation Rate Ratio (c/μ) As Molecular Adaptation Test Beyond Ka/Ks: A SARS-COV-2 Case Study. **Journal of Molecular Evolution, 2025**. DOI: 10.1007/s00239-025-10248-6

2024:

7. Marques, T. J. S.; Salvador, D.; Oliveira, H.; Serra, V. V.; Paradis, N.; Wu, C.; Silva, V. L. M.; Ramos, C. I. V. New acridone derivatives to target telomerase and oncogenes - an anticancer approach. RSC Med Chem 2025. DOI: 10.1039/d4md00959b.
8. Muhammad - Arba, A. A., Ruslin Ruslin, Chun Wu, Wa Ode Yentri Putia Ningtiyas Darmin. Docking-Based Virtual Screening to Identify the Cysteine Protease Falcipain-2 Inhibitors of Plasmodium Falciparum. ***MOLEKUL* 2024**. 19, 1, 406-416 https://doi.org/10.20884/1.jm.2024.19.3.7376

9. Paradis, N.; Wu, C. Enhanced Detection and Molecular Modeling of Adaptive Mutations in SARS-CoV-2 Coding and Non-Coding Regions Using the c/μ Test. **Virus Evolution, 2024**.10 (1), veae089 https://doi.org/10.1093/ve/veae089

10. A.I. Uba, N.J. Paradis, C. Wu, G. Zengin, Computational analysis of natural compounds as potential phosphodiesterase type 5A inhibitors, **Computational Biology and Chemistry**, (2024) 113, 108239 https://doi.org/10.1016/j.compbiolchem.2024.108239

11. Justin Carbone, Nicholas J. Paradis, Dylan Brunt and Chun Wu. Binding Mechanism of Active Form of Molnupiravir to RdRp of SARS-CoV-2 and Designing Potential Analogues: Insights from Molecular Dynamic Simulations. **ACS Omega**, 2024, 9(40), 41583-41598 DOI: 10.1021/acsomega.4c05469

12. Moura, N. M. M.; Guedes, S.; Salvador, D.; Oliveira, H.; Alves, M. Q.; Paradis, N.; Wu, C.; Neves, M. G. P. M. S.; Ramos, C. I. V., Oncogenic and telomeric G-quadruplexes: Targets for porphyrin-triphenylphosphonium conjugates. ***International Journal of Biological Macromolecules* 2024**, 277, 134126. https://doi.org/10.1016/j.ijbiomac.2024.134126

13. Nicholas J. Paradis, Austin Clark, Hunter Gogoj, Timothy D. Vaden,* and **Chun Wu*** Substituting K+ for Imidazolium-based Ionic Liquids to Stabilize a c-MYC DNA G-Quadruplex: A Spectroscopy-Molecular Dynamics Simulation Dual Approach, **Journal of Molecular Liquids,** 2024 124407 https://doi.org/10.1016/j.molliq.2024.124407

14. Hetanshi Choksi, Justin Carbone, Nicholas Paradis, Lucas Bennett, Candice Bui-Linh, **Chun Wu**, Novel Inhibitors to MmpL3 Transporter of Mycobacterium tuberculosis by Structure-based High Throughput Virtual Screening and Molecular Dynamics Simulations, **ACS Omega**, 2024 9, 13782−13796 https://doi.org/10.1021/acsomega.3c08401

15. Abdullahi Ibrahim Uba, Mariya Hryb, Mursalin Singh, Candice Bui-Linh, Annie Tran, Jiancarlo Atienza, Sarah Misbah, Xiaoyang Mou* and **Chun Wu***, Novel potential inhibitors of histone deacetylase 6 identified using structure-based virtual screening, molecular dynamics simulation, enzyme inhibition assay, and cell viability assay, **Life Sciences,** 2024, 338,122395 https://doi.org/10.1016/j.lfs.2023.122395

16. Muhammad Arba, Sri Wahyuli, Arfan, Setyanto Tri Wahyudi, and Chun Wu*, Computational Study of Binding of Oseltamivir to Neuraminidase Mutants of Influenza A Virus, **Journal of Applied Pharmaceutical Science,** 2024 **,** 14(02):239-254 https://doi.org/10.7324/JAPS.2024.147448

2023:

17. Abdullahi Ibrahim Uba, Nicholas Joseph Paradis, **Chun Wu**, Gokhan Zengin, Phenolic compounds as adenosine deaminase inhibitors: binding propensity and interaction analyses using docking and molecular dynamics simulation coupled with MM/GBSA calculations, **Amino Acids,** 2023**,** 55, 1729–1743 https://doi.org/10.1007/s00726-023-03310-4

18. Comfort A. Boateng ,Ashley N. Nilson ,Rebekah Placide ,Mimi L. Pham ,Franziska M. Jakobs ,Noelia Boldizsar ,Scot McIntosh ,Leia S. Stallings ,Ivana V. Korankyi ,Shreya Kelshikar ,Nisha Shah ,Diandra Panasis ,Abigail Muccilli ,Maria Ladik ,Brianna Maslonka ,Connor McBride ,Moises Ximello Sanchez ,Ebrar Akca ,Mohammad Alkhatib ,Julianna Saez ,Catherine Nguyen ,Emily Kurtyan ,Jacquelyn DePierro ,Raymond Crowthers, **Dylan Brunt**, Alessandro Bonifazi ,Amy H. Newman ,Rana Rais ,Barbara S. Slusher ,R. Benjamin Free ,David R. Sibley ,Kent D. Stewart ,**Chun Wu** ,Scott E. Hemby ,Thomas M. Keck, Pharmacology and Therapeutic Potential of Benzothiazole Analogues for Cocaine Use Disorder, **Journal of Medicinal Chemistry,** 2023, 66, 17, 12141–12162 https://doi.org/10.1021/acs.jmedchem.3c00734

19. Dean, Emily; Dominique, AnneMarie; Palillero, Americus; Wu, Chun, To Probe Activation mechanism of agonist DPI-287 to Delta Opioid Receptor and to Identify Novel Agonists using Ensemble-based Virtual Screening with Molecular Dynamics Simulations, **ACS Omega**, 2023, 8, 36, 32404-32423 https://doi.org/10.1021/acsomega.3c01918

20. Carbone, Justin; Paradis, Nicholas; Bennett, Lucas;Alesiani, Mark; Hausman, Katherine; Wu, Chun, Inhibition mechanism of anti-TB drug SQ109: Blocking water passing and TMM entry of Mycobacterium tuberculosis MmpL3 transporter, **Journal of Chemical Information and Modeling,** 2023, 63, 16, 5356–5374 https://doi.org/10.1021/acs.jcim.3c00616

21. Uba, Abdullahi Ibrahim and Bui-Linh, Candice and Thornton, Julianne and Olivieri, Michael and **Wu, Chun**, Computational Analysis of Drug Resistance of Taxanes Bound to Human B-Tubulin Mutant (D26E). **Journal of Molecular Graphics and Modelling**. 2023, 123, 108503 https://doi.org/10.1016/j.jmgm.2023.108503 [2023 Journal Impact Factor = 2.9 ; citations =]

22. Muhammad Arba, Aprilia Surya Ningsih, La Ode Santiaji Bande, Setyanto Tri Wahyudi, Candice Bui-Linh, Chun Wu, and Amir Karton, Computational Insights into the Binding of Pimodivir to the Mutated PB2 Subunit of the Influenza A Virus, **Molecular Simulation.** 2023, 49:10, 1031-1043, [2023 Journal Impact Factor = 2.9 ; citations =] https://doi.org/10.1080/08927022.2023.2210690

23. **Wu, C***, Paradis N., Lakernick P., Hryb M. To decipher the molecular evolution nature of SARS-CoV-2 by examining the variation of the substitution rates within its genome. **Computational Biology and Medicine**. 2023, 153, 106522 [2022 Journal Impact Factor = **6.69**, Citations=]
https://doi.org/10.1016/j.compbiomed.2022.106522

2022

24. Uba, A, Chea, J., Hoag H., Hryb, M, Bui-Linh, C, **Wu, C***, Binding of a positive allosteric modulator CDPPB to metabotropic glutamate receptor type 5 (mGluR5) probed by all-atom molecular dynamics simulations, **Life Sciences** 2022, 309, 15, 121014 [2022 Journal Impact Factor = **6.78** , Citations=1]
https://doi.org/10.1016/j.lfs.2022.121014

25. Uba, A, **Wu. C***, Chapter: Potential competitive inhibitors of SHP-2 identified by structure-based virtual screening and molecular dynamics simulation, **ACS book**: "Physical Chemistry Research at Undergraduate Institutions" 2022, chapter 8, 123-143
https://doi.org/10.1021/bk-2022-1428.ch008

26. Paradis, N. J.; Clark, A.; Gogoj, H.; Lakernick, P. M.; Vaden, T. D.; **Wu, C*.** To probe the binding of TMPyP4 to c-MYC G-quadruplex with in water and in imidazolium-based ionic liquids using spectroscopy coupled with molecular dynamics simulations. **Journal of Molecular Liquids.** 2022 ; 365:120097. [2022 Journal Impact Factor = **6.21,** Citations=]
https://doi.org/10.1016/j.molliq.2022.120097.

27. Dean, E.; Kumar, V.; McConnell, A.; Pagnoncelli, I. B.; **Wu, C***., To probe the activation mechanism of the Delta opioid receptor by an agonist ADL5859 started from inactive conformation using molecular dynamic simulations. **Journal of Biomolecular Structure and Dynamics** 2022, 1-18.
[2022 Jounal Impact Factor = **3.392**, Citations=]
https://doi.org/10.1080/07391102.2022.2107074

28. Uba AI, Aluwala H, Liu HG, **Wu C***. Elucidation of partial activation of cannabinoid receptor type 2 and identification of potential partial agonists: Molecular dynamics simulation and structure-based virtual screening. **Computational Biology and Chemistry**. 2022 99:107723. [2022 Journal Impact Factor = **3.737,** Citations=] https://doi.org/10.1016/j.compbiolchem.2022.107723.

29. Uba AI, **Wu C***. Identification of potential antagonists of CRF1R for possible treatment of stress and anxiety neuro-disorders using structure-based virtual screening and molecular dynamics simulation. **Computational Biology and Chemistry**. 2022:107743. [2022 Journal Impact Factor = **3.737,** Citations=] https://doi.org/10.1016/j.compbiolchem.2022.107743.

30. DJ Brunt, PM Lakernick, **C. Wu***, Discovering new potential inhibitors to SARS-CoV-2 RNA dependent RNA polymerase (RdRp) using high throughput virtual screening and molecular dynamics simulations, **Scientific Reports**, 2022. 12, 19986,
[2022 Journal Impact Factor = **4.996**, Citations=] https://doi.org/10.1038/s41598-022-24695-4

31. M. Arba, N. Paradis, S.T. Wahyudi, D.J. Brunt, K.R. Hausman, P.M. Lakernick, M. Singh, **C. Wu***, Unraveling the binding mechanism of the active form of Remdesivir to RdRp of SARS-CoV-2 and designing new potential analogues: Insights from molecular dynamics simulations, **Chemical Physics Letters**, 799 (2022) 139638. [2022 Journal Impact Factor = **2.719** , Citations=]
https://doi.org/10.1016/j.cplett.2022.139638

32. M. Arba, S.T. Wahyudi, M.S. Zubair, D. Brunt, M. Singh, **C. Wu***, Binding of GS-461203 and Its Halogen Derivatives to HCV Genotype 2a RNA Polymerase Drug Resistance Mutants, **Scientia Pharmaceutica**, (2022) 90(2), 26. [2022 Journal Impact Factor = **4.94** , Citations=]
https://doi.org/10.3390/scipharm90020026

33. S. Liao, M.J. Pino, C. Deleon, M. Lindner-Jackson, **C. Wu***, Interaction analyses of hTAAR1 and mTAAR1 with antagonist EPPTB, **Life Sciences**, 300 (2022) 120553. [2022 Journal Impact Factor = **6.78** , Citations=] https://doi.org/10.1016/j.lfs.2022.120553

34. Patel, D. C.; Hausman, K. R.; Arba, M.; Tran, A.; Lakernick, P. M.; **Wu, C**.*, Novel inhibitors to ADP ribose phosphatase of SARS-CoV-2 identified by structure-based high throughput virtual screening and molecular dynamics simulations. ***Computers in Biology and Medicine* 2022**, 140, 105084.
[2022 Journal Impact Factor = **6.69,** Citations=**3**]
https://doi.org/10.1016/j.compbiomed.2021.105084

2021:

35. Lupala, C.S.; Kumar, V.; Su, X.-d.; **Wu, C**.; Liu, HG. Computational insights into differential interaction of mammalian angiotensin-converting enzyme 2 with the SARS-CoV-2 spike receptor binding domain. **Computers in Biology and Medicine** 2021, 105017 [2022 Journal Impact Factor = **6.69 ,** Citations=**7**]
https://doi.org/10.1016/j.compbiomed.2021.105017

36. Patel, A. Y.; Clark, A. K.; Paradis, N. J.; Amin, M.; Vaden, T. D**.; Wu, C.;** Caputo, G. A., Effects of Ionic Liquids on Laccase from Trametes versicolor. **Biophysica** 2021, 1, 429-444.
[2022 Journal Impact Factor = **4.033**, Citations=**1**]
https://doi.org/10.3390/biophysica1040031

37. Kumar, V.; Liu, HG*.; **Wu, C***, Drug Repurposing against SARS-CoV-2 Receptor Binding Domain using Ensemble-based Virtual Screening and Molecular Dynamics Simulations, **Computers in Biology and Medicine,** 2021**,** 135, 104634, [2022 Journal Impact Factor = **6.69 ,** Citations=**9**]
https://doi.org/10.1016/j.compbiomed.2021.104634

38. Leung, L.; Liao, SY; **Wu, C.*,** To probe the binding interactions between two FDA approved migraine drugs (Ubrogepant and Rimegepant) and calcitonin-gene related peptide receptor (CGRPR) using molecular dynamics simulations, **ACS Chemical Neuroscience,** 2021, 12(14), 2629-2642
[2022 Journal Impact Factor = **5.78,** Citations=]
https://doi.org/10.1021/acschemneuro.1c00135

39. Uba, AI; Scorese, N.; Dean, E.; Liu, HG; **Wu, C.***, Activation Mechanism of Corticotrophin Releasing Factor Receptor Type 1 Elucidated Using Molecular Dynamics Simulation, **ACS Chemical Neuroscience**, 2021, 12(9), 1674-1687, [2022 Journal Impact Factor =**5.78,** Citations=**5**]
https://doi.org/10.1021/acschemneuro.1c00126

40. DeStefano, I.; DeStefano G.; Paradis NJ; Patel R.; Clark AK; Gogoj H.; Singh G.; Jonnalagadda KS; Patel AY; **Wu C**.; Caputo GA; Vaden TD Thermodynamic destabilization of azurin by four different tetramethylguanidinium amino acid ionic liquids, **International J of Biological Macromolecules,** 2021, 180,355-364, [2022 Journal Impact Factor =**8.025,** Citations=**4**]
https://doi.org/10.1016/j.ijbiomac.2021.03.090

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