CHUN WU
Departments of Chemistry & Biochemistry and Biological & Biomedical Sciences
College of Science and Mathematics
Rowan University
201 Mullica Hill Road, Glassboro, NJ 08028,
Tel: (856) 256-5462, Fax: (856) 256-4478
e-Mail: wuc@rowan.edu
Web: http://users.rowan.edu/~wuc

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 the Biological Biomedical Sciences at Rowan University. He obtained his PhD from University of Delaware where he worked on force field development and conducted molecular dynamics simulations of amyloidogenic peptides. He then trained at the University of California Davis and Santa Barbara as a postdoctoral researcher developing structural model of amyloidogenic peptides oligomers. At Rowan, using genomic datasets his lab is developing a novel evolution theory (near-neutral balanced selection theory/NNBST) not only to best explain the molecular evolution of SARS-COV-2 and other pathogens but also to accurately identify hotspots in their genome for developing first/next generation vaccines and drugs to treat these infectious diseases; using molecular docking, homology modeling and molecular dynamics simulations, his computer aided drug design (CADD) lab is investigating the binding interactions between various protein receptors and ligands toward novel drug design. Working collaboratively with experimental groups, the Wu lab aims to discover novel protein receptors and small molecules as potential anti-cancer agents, antiviral agents, anti-neural-disorder agents, and to optimize ionic liquids for protein and nucleic acid stabilization. With over 100 peer-reviewed publications and a total awarded external grant of $1.5 million and 3.3 million CPU hours as a PI and co-PI, he has achieved a h-index of 37 and total citations of 9620+. His contributions to the field of computational biochemistry, molecular modeling and simulation and CADD are recognized by his peers. He has been invited to present at national and international meetings, and top Chinese institutes, and he was named the World Class Professor by the Indonesia Ministry of Education and Culture in 2021, his CADD lab won the Rowan University Breakthrough of the Year Award (2023). In addition to his research, Chun is also passionate about teaching and mentoring students at both the undergraduate and graduate level. At CSRC, he co-supervised two postdocs (Uba and Vikash), Uba is now an Assistant Professor at the Department of Molecular Biology and Genetics, Istanbul AREL University, Istanbul, Turkey since February 2023. At Rowan, he has supervised over 34 MS graduate students and 120 undergraduates in research leading to over 28+23 publications and 69+83 posters.

EDUCATION

2005	Ph. D.	Computational Chemistry	**University of Delaware**, Newark, DE
2005	M. S.	Computer Science	**University of Delaware**, Newark, DE
1999	M. S.	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

(Total awarded external grants **$1.55 million** as PI and Co-PI)

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.

2017-2024 Sole PI: **C WU**, *Request of computational time for a bioinformatics course in Fall* National Science Foundation: **ACCESS/BIO230145, 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

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

2022-2025 Faculty Mentor, **C Wu**, NIH, Bridges to the Baccalaureate, 2022-2025, 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 (94 total, h-index 37, total citations 9422+)

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

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

2024:

1. 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, **ACS Omega,** 2024 **under preparation**

2. 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**, 2024 under review

3. 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

4. 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 https://doi.org/10.1021/acsomega.3c08401

5. 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

6. 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:

7. 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

8. 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

9. 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

10. 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

11. 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 =]

12. 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

13. **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

14. 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

15. 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

16. 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.

17. 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

18. 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.

19. 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.

20. 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

21. 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

22. 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

23. 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

24. 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:

25. 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

26. 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

27. 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

28. 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

29. 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

30. 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

31. Patel, A. Y.; Jonnalagadda, K. S.; Paradis, N.; Vaden, T. D.; **Wu, C**.; Caputo, G. A., Effects of Ionic Liquids on Metalloproteins. **Molecules** 2021, 26(2), 514. PMID: 33478102; PMCID: PMC7835893
https://doi.org/10.3390/molecules26020514 [2022 Journal Impact Factor =**4.927,** Citations=**17**]

32. Arba, M.; Wahyudi, S. T.; Brunt, D. J.; Paradis, N.; **Wu, C.***, Mechanistic insight on the remdesivir binding to RNA-Dependent RNA polymerase (RdRp) of SARS-cov-2. **Computers in Biology and Medicine** 2021, 129, 104156.. PMID: 33260103; PMCID: PMC7691827 [2022 Journal Impact Factor = **6.69**, Citations=**17**]
https://doi.org/10.1016/j.compbiomed.2020.104156

33. S Liao, K Tan, C Floyd, D Bong, MJ Pino Jr, **C Wu*.** Probing biased activation of mu-opioid receptor by the biased agonist PZM21 using all atom molecular dynamics simulation**, Life Sciences** 2021, 269, 119026.. PMID: 33444617 [2022 Journal Impact Factor = **6.78** , Citations=**4**]
https://doi.org/10.1016/j.lfs.2021.119026

2020:

34. Arba, M.; Nur-Hidayat, A.; Usman, I.; Yanuar, A.; Wahyudi, S. T.; Fleischer, G.; Brunt, D. J.; **Wu, C*.**, Virtual Screening of the Indonesian Medicinal Plant and Zinc Databases for Potential Inhibitors of the RNA-Dependent RNA Polymerase (RdRp) of 2019 Novel Coronavirus. **Indonesian Journal of Chemistry**; 2020, 20(6),1430-1440 [2022 Journal Impact Factor = **1.287**, Citations=**5**]
https://doi.org/10.22146/ijc.56120

35. Cheng, R.; **Wu, C***.; Cao, Z*.; Wang, B*., QM/MM MD simulations reveal an asynchronous PCET mechanism for nitrite reduction by copper nitrite reductase. **Physical Chemistry Chemical Physics 2020**, 22, 20922-20928. PMID: 32924054 [2022 Journal Impact Factor = **3.676** , Citations=**4**]
https://doi.org/10.1039/d0cp03053h

36. Sullivan, H.-J.; Chen, B.; **Wu, C*.**, A molecular dynamics study on the binding of an anti-cancer DNA G-quadruplex stabilizer, CX-5461, to human telomeric, cKIT-1, and c-Myc G-quadruplexes and a DNA duplex. **Journal of Chemical Information and Modeling 2020**. 60,10, 5203-5224,. PMID: 32820923

https://doi.org/10.1021/acs.jcim.0c00632 [2022 Journal Impact Factor = **6.162,** Citations=**8**]

37. Chen, B.; Fountain, G.; Sullivan, H.-J.; Paradis, N.; **Wu, C***., To probe the binding pathway of a selective compound (D089-0563) to c-MYC Pu24 G-quadruplex using free ligand binding simulations and Markov state model analysis. **Physical Chemistry Chemical Physics 2020,** 22, 22567-22583 PMID: 33000836 [2022 Journal Impact Factor = **3.676,** Citations=**4**]
https://doi.org/10.1039/d0cp03863f

38. Kumar, V.; Hoag, H.; Sader, S.; Scorese, N.; Liu, HG*.; **Wu, C***., GDP Release from the Open Conformation of Gα Requires Allosteric Signaling from the Agonist-Bound Human β2 Adrenergic Receptor. **Journal of Chemical Information and Modeling 2020**, 60, 4064-4075,. PMID: 32786510
https://doi.org/10.1021/acs.jcim.0c00432 [2022 Journal Impact Factor = **6.162,** Citations=**3**]

39. Cairns, T. M.; Atanasiu, D.; Saw, W. T.; Lou, H.; Whitbeck, J. C.; Ditto, N. T.; Bruun, B.; Browne, H.; Bennett, L.; **Wu, C.;** Krummenacher, C.; Brooks, B. D.; Eisenberg, R. J.; Cohen, G. H., Localization of the Interaction Site of Herpes Simplex Virus Glycoprotein D (gD) on the Membrane Fusion Regulator, gH/gL. **Journal of Virology** 2020, 94, e00983-20. PMID: 32759318; PMCID: PMC7527043
https://doi.org/10.1128/JVI.00983-20 [2022 Journal Impact Factor = **4.501,** Citations=**10**]

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104. Sui W, **Wu C**, Li YQ (2000) *"Rapid simultaneous determination of four anthracene derivatives using a single non-linear variable-angle synchronous fluorescence spectrum."* **Fresenius' Journal of Analytical Chemistry** 368: 669-675. [2022 Impact Factor = **1.237**, Citations=**17**] PMID: 11227546 https://doi.org/10.1007/s002160000551

† Contribute equally
* Corresponding authors

LIST OF ORAL PRESENTATION IN INTERNATIONAL/NATIONAL/REGIONAL/LOCAL MEETINGS AND INVITED TALKS SINCE JOINING ROWAN (Undergraduate Students Underlined)

1. **C. Wu**, Paradis, N, , Generalized c/μ Ratio Test for Detecting Molecular Adaptation: Beyond the conventional Ka/Ks Ratio test without Assuming Synonymous Site Neutrality or Limitation to Translated Regions, Intelligent Systems for Molecular Biology **(ISMB 2024**), Track: EvolCompGen, 2024, July 11-16, 2023**,** Montreal, Canda
2. **C. Wu**, The 1st "Near-Neutral Balanced Selectionist Theory (NNBST): a quantitative evolution theory to explain genomic evolution of SARS-CoV-2 and Other Deadly Viruses and its application in vaccine and drug development", **Halu Oleo International Conference on Pharmacy, Health and Applied Sciences 2023**" with theme "Converging Frontiers: Andvancing Healthcare Solution through Pharmaceutical Chemistry and Technology", November 20, 2023.
3. **C. Wu,** Advances in Drug Discovery and Development, **Technology Networks**, Webinar, September 27-28, 2023
4. **C. Wu**, Teach computer-aided drug design (CADD) in the upper-level bioinformatics/biochemistry /molecular modeling courses using schrodinger package**, Schrodinger's Educators Week 2023**, June 15, 2023, New York
5. **C. Wu,** A High-Throughput Virtual Screening Approach to Identifying Novel SARS-CoV-2 Inhibitors, **Technology Networks**, Webinar, March 30, 2023
6. Hryb, M., Davis L., Lao S., Daringer N., Mou XY, and **Wu. C.** To probe activation mechanism of HER2 directed Chimeric T-Cell Receptor (CAR) by antigen using homology modeling and all-atom molecular dynamics simulation by Anton2, **the ACS Fall 2023 National Meeting & Expo**, San Francisco, CA, August 13-17, 2023.
7. **C.Wu,** Bennet L., Paradis, N., Carbone J. Alesiani M. Hausman K. Inhibition mechanism of anti-TB drug SQ109: Blocking water passing and TMM entry of Mycobacterium tuberculosis MmpL3 transporter**, the ACS Fall 2023 National Meeting & Expo**, San Francisco, CA, August 13-17, 2023.
8. **C. Wu**, Paradis, N, Lakernick P, Hryb M., the L-shaped distribution of the relative substitution rate (c/u) observed for SARS-COV-2 genome, inconsistent with the selectionist theory, the neutral theory and the nearly neutral theory but a near-neutral balanced selection theory, Intelligent Systems for Molecular Biology/European Conference On computational Biology/ECCB **(ISMB/ECCB**), Track: EvolCompGen, 2023, July 23-27, 2023**,** Lyon, France
9. **Chun Wu**, Abdullahi Ibrahim Uba, John Chea, Hannah Hoag, Mariya Hryb, and Candice Bui-Linh, Binding of a positive allosteric modulator CDPPB to metabotropic glutamate receptor type 5 (mGluR5) probed by all-atom molecular dynamics simulations**, the ACS Spring 2023 National Meeting & Expo,** March 26 - 30**, 2023**
10. **C. Wu,** Arba, M., Paradis, N., Wahyudi ST, Brunt DJ, Hausman KR, Lakernick P., Mursalin Singh, 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. **the ACS Fall 2022 National Meeting & Expo**, August 21 - 25, **2022**.
11. **C. Wu,** Brunt DJ, Lakernick P. Discovering new potential inhibitors to SARS-CoV-2 RNA dependent RNA polymerase (RdRp) using high throughput virtual screening and molecular dynamics simulations. **the ACS Fall 2022 National Meeting & Expo**, August 21 - 25, **2022**.

12. **C. Wu,** Darriger NM, Hryb M., Leah D. and Lao S. Structure and dynamics of HER2 directed Chimeric T-Cell Receptor (CAR) using homology modeling and all-atom molecular dynamics simulation with explicit solvent, **the ACS Fall 2022 National Meeting & Expo**, August 21 - 25, **2022**.
13. Al Uba, HG Liu, **C. Wu** "Novel potential inhibitors of histone deacetylase 6 identified using structure based virtual screening and molecular dynamics simulation", **the ACS Spring 2022 National Meeting & Expo**, March 20-24, **2022**.
14. H. Aluwala, **C. Wu** "High throughput virtual screening to identify small molecule agonists for glucagon-like peptide-1 receptor", **the ACS Spring 2022 National Meeting & Expo**, March 20-24**, 2022**.
15. Al Uba, H. Aluwala, HG Liu, **C. Wu "** Probing partial activation of cannabinoid receptor type 2 and identification of novel partial agonist by structure-based virtual screening and molecular dynamics simulation", **the ACS Spring 2022 National Meeting & Expo**, March 20-24, **2022**.
16. E. Dean, V. Kumar, A. McConnell, I. Pagnoncelli, **C. Wu "** To probe the activation mechanism of the delta opioid receptor by an agonist ADL5859 started from an inactive conformation using molecular dynamic simulations**", the ACS Spring 2022 National Meeting & Expo**, March 20-24, **2022**.
17. L. Bennett**,** and **C.Wu** "Probe the inhibition mechanism of SQ109, an investigative inhibitor of the Mycobacterium tuberculosis MmpL3 transporter protein using molecular dynamics simulations", **the ACS Fall 2021 National Meeting & Expo**, August 22-26, **2021**.
18. A. Uba**,** N. Scorese, E. Dean, H.G. Liu, **C Wu** " Activation mechanism of corticotrophin releasing factor receptor Type 1 elucidated using molecular dynamics simulation" **the ACS Fall 2021 National Meeting & Expo**, August 22-26, **2021**.
19. L Leung**, C. Wu** "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" **the ACS Fall 2021 National Meeting & Expo**, August 22-26, **2021**.
20. N.J. Paradis**, C. Wu** "Probe structure and dynamics of E-protein of both SARS-CoV-2 and SARS-CoV-1, implication on the virulence increase due to the two key mutations E69R and ΔG70" **the ACS Fall 2021 National Meeting & Expo**, August 22-26, **2021**.
21. S.Y Liao, M. Pino**, C. Wu** "Analysis of human TAAR1 and mouse TAAR1 with Antagonist EPPTB toward selective ligands to hTAAR1 using homology modeling, docking and molecular dynamics simulation and virtual screening", **the ACS Fall 2021 National Meeting & Expo**, August 22-26**, 2021**.
22. **Wu C,** E. Dean "Molecular dynamics simulations of the δ-opioid receptor agonist and antagonist to suggest conformational change from inactive to active states", **the ACS Spring 2020 National Meeting & Expo**, March 22-26, **2020**. (Converted into on-line slide presentation, due to covid-19 pandemics)
23. **Wu C** "molecular dynamics simulations" in Summer Workshop "Theoretial and computation biology: from moleuces to systems, **Songshan Lake in Dongguan**, Aug 1-4, **2019**
24. **Wu C** "Computer Aided Drug Design (CADD) targeting Virus, cancers and signal transduction pathways", School of Pharmaceutical Sciences, **Xiamen University**, August 15**, 2019** Host: Prof. WANG binju
25. **Wu C** "Binding of BRACO19 to a telomeric G-quadruplex DNA probed by all-atom molecular dynamics simulations with explicit solvent", **the 2019 Middle Atlantic Regional Meeting**, Baltimore, MD, May 30 - June 1, 2019.
26. **Wu C** "Binding of EMICORON to human vascular endothelial growth factor receptor-2 (vegfr-2) G-quadruplex probed by homology modeling and all-atom molecular dynamics simulations", SESSION: Molecular Mechanics: Recent Advances in Simulations of Nucleic Acids", **the ACS Spring 2019 National Meeting & Expo**, New Orleans, LA, March 18-22**, 2019**.
27. **Wu C "**Computer Aided Drug Design (CADD) targeting Virus, cancers and signal transduction pathways**" Department of Physics, Fudan University**, August 3**, 2018**, Host: Prof. WEI Guanghong
28. **Wu C** "Computer Aided Drug Design (CADD) targeting Virus, cancers and signal transduction pathways" **College of Pharmaceutical Sciences, Zhejiang University**, August 2, **2018**, Host: Prof. HOU Tingjun
29. **Wu C** "Computer Aided Drug Design (CADD) targeting Virus, cancers and signal transduction pathways" **Department of Chemistry, Yunnan University**, July 31, **2018**, Host: Prof. XU SiChuan

30. **Wu C** "Computer Aided Drug Design (CADD) targeting Virus, cancers and signal transduction pathways" State Key Laboratory of Trauma, Burn and Combined Injury, Department of Trauma Surgery, **Daping Hospital, Army Medical University**, Chong Qing, July 27, **2018**, Prof. XU Xiang
31. **Wu C** "Computer Aided Drug Design (CADD) targeting Virus, cancers and signal transduction pathways" Department of Chemistry, Sichuan University, July 26, **2018**, Prof. PU Xuemei
32. **Wu C** "Computer Aided Drug Design (CADD) targeting Virus, cancers and signal transduction pathways", **School of Pharmaceutical Sciences, Guangzhou Medical University**, July 25, **2018**, Prof. GAO Hui
33. **Wu C** "Computer Aided Drug Design (CADD) targeting Virus, cancers and signal transduction pathways", **School of Pharmaceutical Sciences, Sun Yat-Sen University**, July 24, **2018**, Host: Prof WU Ruibo
34. **Wu C** "Computer Aided Drug Design (CADD) targeting Virus, cancers and signal transduction pathways", **School of Pharmaceutical Sciences, Xiamen University**, July 23, **2018** Host: Prof. LIU Wen
35. **Wu C** "Computer Aided Drug Design (CADD) targeting Virus, cancers and signal transduction pathways" Department of Chemistry, **Xiamen University**, July 23, **2018** Host: Prof. TAN Kai
36. **Wu C** "Computer Aided Drug Design (CADD) targeting Virus, cancers and signal transduction pathways", School of Chemistry and Chemical Engineering, **Nanjing University**, July 20, **2018**, Prof. MA Jing
37. **Wu C** "Computer Aided Drug Design (CADD) targeting Virus, cancers and signal transduction pathways" Center of Quantitative Biology, **Beijing University**, July 18, **2018**, Host: Prof. LAI luhua, SONG Hao
38. **Wu C** "Computer Aided Drug Design (CADD) targeting Virus, cancers and signal transduction pathways" Department of Chemistry, **Beijing Normal University**, July 18, **2018**, Host: Prof. GAO Lianghui
39. **Wu C** "Computer Aided Drug Design (CADD) targeting Virus, cancers and signal transduction pathways" **Beijing Computational Research Sciences Center (**CRSC), July 17, **2018**, Host: Prof. LIU haiguang
40. **Wu C** "Computer Aided Drug Design (CADD) targeting Virus, cancers and signal transduction pathways" Department of Physics, **Beijing University of Posts and Telecomunications,** July 16, **2018**, Host: Prof. LAN Yueheng
41. **Wu C,** Mullholland K "Binding of TMPyP4 to RNA G-Quadruplex Containing ALS and FTD Related G4C2 Repeat Probed by All-Atom Molecular Dynamics Simulations with Explicit Solvent", SESSION: Molecular Mechanics, **the 255th ACS National Meeting**, New Orleans, LA, March 18-22**, 2018**.
42. **Wu C** "Computer Aided Drug Design (CADD) targeting cancers and signal transduction pathways", **Dept. of Chemistry & Physical Sciences, Pace University**, February 28, **2018**
43. Alexandra Campbell and **Chun Wu,** *"Binding of Anticancer Chelerythrine to DNA G-quadruplexes Promoters (BCL2, KRAS and VEGF) Using Molecular Dynamics Simulations"*, MCB **2018** Fall Symposium, December 8, 2018, Science Hall, Room 126
44. Stephen Ahwin, John Alviar and **Wu C** "Survey of GPCR Structures for Understanding Activation Mechanism & Virtual Screening" MCB **2018** Fall Symposium, December 8, 2018, Science Hall, Room 126
45. Sader S, **Wu C** *"In silico Visioning of G Protein-GDP Complex Communications with GPCR Bound to Different Ligands Using Molecular Dynamic Simulations"*, SESSION: Membrane Proteins: Structure, Activity & Drug Development, **the 254th ACS National Meeting in Washington**, DC, August 20-24, 2017.
46. Mullholland K, Siddiquei F, **Wu C** *"Binding modes and pathway of RHPS4 to human telomeric G-quadruplex and duplex DNA probed by all-atom molecular dynamics simulations with explicit solvent"*, SESSION: Physical Chemistry Research at Undergraduate Institutions, **the 254th ACS National Meeting in Washington**, DC, August 20-24, 2017.
47. **Wu C,** Machireddy B. ***"****Probing the binding mechanism of BRACO19 to parallel quadruplexes from human telomeric DNA using molecular dynamics simulation with a free ligand", SESSION: Molecular Mechanics, **the 254th ACS National Meeting in Washington**, DC, August 20-24, 2017.*
48. Sader S, Anant K, **Wu C** *"Probe activation mechanism of 6TM variants of human μ-opioid receptor by morphine derivative (IBNtxA) using all-atom molecular dynamics simulation with explicit membrane" the platform session of Membrane Receptors & Signal Transduction, **the Biophysical Society 61st Annual Meeting**,NewOrleans, Louisiana, Feb. 11 – 15, 2017*

LIST OF POSTER PRESENTATION IN ITERNATIONAL/NATIONAL/REGIONAL/LOCAL MEETINGS SINCE JOINING ROWAN (UNDERGRADUATE STUDENTS UNDERLINED)

49. Nicholas Paradis, **Chun Wu,** c/μ Relative Substitution Rate Test Infers Synonymous Mutations Also Drive Zika Virus Molecular Evolution, Variant Interpretation, Intelligent Systems for Molecular Biology (**ISMB 2024**), 2024, July 11-16, 2023, Montreal, Canda
50. Nicholas Paradis, **Chun Wu,** Development of an In-silico Sequence and Structure-based Virtual Screening Workflow to Develop Novel Small Molecular Inhibitors Against Wild-Type and Mutant Zika Virus NS5 Polymerase, Structural Bioinformatics and Computational Biophysics, Intelligent Systems for Molecular Biology (**ISMB 2024**), 2024, July 11-16, 2023, Montreal, Canda
51. Khushi Jain and Chun Wu, Enterovirus D68: Embracing Near-Neutral Balanced Selectionist Theory (NNBST) Over Mainstream Theories, Evolution and Comparative Genomics, Intelligent Systems for Molecular Biology (**ISMB 2024**), 2024, July 11-16, 2023, Montreal, Canda
52. Nicholas J. Paradis, Chun Wu, Phillip M. Lakernick and Mariya Hyrb, Near-Neutral Balanced Selection Theory (NNBST): Implication on the molecular evolution of SARS-CoV-2 and Zika virus, **Annual ACS Rowan Student Research Symposium**, December 1, 2023
53. Samee Khan, Clement Vu, Mariya Hryb and Chun Wu*, Validation of Novel Evolution Theory, NNBST, against Ebola Virus and its application to identify Mutations Causing Vaccine Escape and Drug Resistance, **Annual ACS Rowan Student Research Symposium**, December 1, 2023
54. Khushi Jain, **Chun Wu**, Understanding the Molecular Evolution of Enterovirus D68: A Near-Neutral Balanced Selectionist Theory (NNBST) Perspective and Implications for Drug and Vaccine Development, **Annual ACS Rowan Student Research Symposium**, December 1, 2023
55. Hetanshi Choksi, Mariya Hryb, and **Chun Wu***, Identifying Mutations Causing Vaccine Escape and Drug Resistance Using NNBST for Monkeypox, **Annual ACS Rowan Student Research Symposium**, December 1, 2023
56. Nishtha Patel, **Chun Wu**, Mumps: Identifying mutations causing vaccine escape and drug resistance, **Annual ACS Rowan Student Research Symposium**, December 1, 2023
57. Priyaben Patel, **Chun Wu**, Unveiling the Molecular Evolution of Respiratory Syncytial Virus: A Near-Neutral Balanced Selectionist Theory (NNBST) Perspective and Implications for Vaccine Development, **Annual ACS Rowan Student Research Symposium**, December 1, 2023
58. Philip Gance, Nicholas Paradis, Abby White, and **Chun Wu**, molecular evolution analysis of zika virus envelope and membrane proteins: implications for vaccine development based on near neutral balanced selection theory, **Annual ACS Rowan Student Research Symposium**, December 1, 2023
59. Drashti Gedia, **Chun Wu**, Unveiling the Dynamics of Measles Virus: A Near-Neutral Balanced Selectionist Theory (NNBST) Perspective and Implications for Vaccine Development, **Annual ACS Rowan Student Research Symposium**, December 1, 2023
60. Lucas Bennett, Hetanshi Choksi, and Chun Wu, To identify Novel Inhibitors to MmpL3 transporter of Mycobacterium tuberculosis using Structure-based High Throughput Virtual Screening and Molecular Dynamics Simulations, Oncology Symposium, the NJ Academic Drug Discovery Consortium, November 16, 2023, Princeton University, Frick Chemistry Labs
61. Justin Carbone, Dylan Brunt, Xiaoyang Mou, Chun Wu, Identifying Novel Nucleotide Inhibitor Alternatives to Molnupiravir for Better Selectivity to RdRP of SARS-CoV-2 using Structural Based Virtual Screening and Molecular Dynamic Simulations, Oncology Symposium**, the NJ Academic Drug Discovery Consortium**, November 16, 2023, Princeton University, Frick Chemistry Labs
62. Emily Dean, Annie Tran, AnneMarie Dominique, Americus Palillero and Chun Wu*, Probing the Activation mechanism of agonist DPI-287 to Delta Opioid Receptor and Novel Agonists to using Ensemble-based Virtual Screening with Molecular Dynamics Simulations, Oncology Symposium, **the NJ Academic Drug Discovery Consortium**, November 16, 2023, Princeton University, Frick Chemistry Labs
63. 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, Oncology Symposium, **the NJ Academic Drug Discovery Consortium**, November 16, 2023, Princeton University, Frick Chemistry Labs

64. 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, Oncology Symposium, **the NJ Academic Drug Discovery Consortium**, November 16, 2023, Princeton University, Frick Chemistry Labs

65. Annie Tran, Nicholas Paradis, and **Chun Wu,** Unveiling the Intricacies of HIV-1's gp120 and gp41 Glycoprotein Envelope Gene Evolution through a Novel Near-Neutral Balance Theory Approach**, 2023 MidAtlantic Bioinformatics Conference**, October 6, 2023, 3501 Civic Center Boulevard Philadelphia, PA 19104

66. Nicholas J. Paradis, Bharat Elango, Hunter St-Pierre and **Chun Wu*,** Does the evolutionary nature of a hemagglutinin and neuraminidase gene from influenza a virus (h3n2) follow a recently proposed molecular evolution theory: near-neutral balanced selectionist theory (NNBST)?**, 2023 MidAtlantic Bioinformatics Conference**, October 6, 2023, 3501 Civic Center Boulevard, Philadelphia, PA 19104

67. Philip Gance, Nicholas Paradis, Abby White, and **Chun Wu,** molecular evolution analysis of zika virus envelope and membrane proteins: implications for vaccine development based on near neutral balanced selection theory,2023 MidAtlantic Bioinformatics Conference, October 6, 2023, 3501 Civic Center Boulevard
Philadelphia, PA 19104

68. Bui-Linh C., Hryb M., Mou XY and **Wu C**. Developing the next generation of EGFR inhibitors using high-throughput virtual screening coupled with molecular dynamics simulations, **the ACS Fall 2023 National Meeting & Expo**, San Francisco, CA, August 13-17, 2023.

69. Paradis, N., Clark A., Lakernick P., Vaden T. **Wu C.**, To probe the binding of TMPyP4 to C-MYC G-quadruplex in water and in imidazolium-based ionic liquids: Strategy towards developing stabilizers for nucleic acid therapeutics, **the ACS Fall 2023 National Meeting & Expo**, San Francisco, CA, August 13-17, 2023.

70. Paradis, N. Bui-Linh C., Hyrb M. Mou XY and **Wu C**., Discovering potential BACE2 inhibitors with favorable pharmacokinetic parameters: A computational approach, **the ACS Fall 2023 National Meeting & Expo**, San Francisco, CA, August 13-17, 2023.

71. Hryb M., Leah D. and Lao S, Darriger NM, Mou XY, **Wu C.** To probe activation mechanism of HER2 directed Chimeric T-Cell Receptor (CAR) by antigen using homology modeling and all-atom molecular dynamics simulation by Anton2, Intelligent Systems for Molecular Biology/European Conference On computational Biology/ECCB (**ISMB/ECCB 2023**), Track: 3DSIG COSI, 2023, July 23-27, Lyon, France TRACK

72. Candice Bui Linh, Mariya Hryb, Mursalin Singh, Abdullahi Ibrahim Uba, Jiancarlo Atienza, Annie Tran, Sarah Misbah, Xiaoyang Mou, and **Chun Wu**, Novel HDAC6 inhibitors for treating triple negative breast cancer identified using structure based virtual screening, molecular dynamics simulation, enzyme inhibition assay, and cell viability assay,**16th Annual Undergraduate Research Symposium William Patterson University**, April 22, 2023

73. Emily Dean, AnneMarie Dominique, Americus Palillero, **Chun Wu**, To probe activation mechanism of agonist DPI-287 to delta opioid receptor and novel agonists to using ensemble-based virtual screening with molecular dynamics simulations, **16th Annual Undergraduate Research Symposium William Patterson University**, April 22, 2023

74. Abdullahi Uba, John Chea, Sarah Halim, Amber Mott, Jasmine Mott, Iman Moosvi, Alicia Petrany, 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**, 16th Annual Undergraduate Research Symposium William Patterson University, April 22, 2023**

75. Candice Bui Linh, Mariya Hryb, Mursalin Singh, Abdullahi Ibrahim Uba,Jiancarlo Atienza, Annie Tran, Sarah Misbah, Xiaoyang Mou, and **Chun Wu**, Novel HDAC6 inhibitors for treating triple negative breast cancer identified using structure based virtual screening, molecular dynamics simulation, enzyme inhibition assay, and cell viability assay**, CSM research day,** April 21 2023

76. Alicia Petrany, and **Chun Wu**, Novel Drug Targets For CSF1R Revealed By High-Throughput Virtual Screening Of Zinc15 Library Compounds, **CSM research day,** April 21 2023
77. Lucas Bennet, Nicholas J. Paradis, Justin Carbone, Mark C. Alesiani, Katherine R. Hausman, and **Chun Wu**, Inhibition Mechanism of antiTB drug SQ109: Allosteric Inhibition of TMM Translocation of Mycobacterium Tuberculosis MmpL3 Transporter, **CSM research day,** April 21 2023
78. Nicholas J. Paradis, Bharat Elango, Hunter St Pierre and **Chun Wu**, Does the Evolutionary Nature of a Hemagglutinin and Neuraminidase Gene from Influenza A Virus (H3N2) Follow a Recently Proposed Molecular Evolution Theory: Near Neutral Balanced Selectionist Theory(NNBST). **CSM research day,** April 21 2023
79. **Chun Wu**, Nicholas J. Paradis, Phillip M. Lakernick and Mariya Hyrb, Debunking old evolution theories, proposing new one (near neutral balanced selection theory/NNBST) using SARS CoV 2 genomic data, **CSM research day,** April 21 2023
80. Candice Bui Linh, Abdullahi Ibrahim Uba, Julianne M Thornton, Michael Oliveieri, and **Chun Wu**, Computational analysis of drug resistance of taxanes bound to human β tubulin mutant (D26E), **CSM research day,** April 21 2023
81. Abdullahi Uba, John Chea, Sarah Halim, Amber Mott, Jasmine Mott, Iman Moosvi, Alicia Petrany, 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**, CSM research day**, April 21 2023
82. Justin Carbone, Dylan Brunt, Xiaoyang Mou, **Chun Wu**, Identifying Novel Nucleotide Inhibitor Alternatives to Molnupiravir for Better Selectivity to RdRP of SARS CoV 2 using Structural Based Virtual Screening and Molecular Dynamic Simulations, **CSM research day,** April 21 2023
83. Emily Dean, AnneMarie Dominique, Americus Palillero**, Chun Wu**, To probe activation mechanism of agonist DPI-287 to delta opioid receptor and novel agonists to using ensemble-based virtual screening with molecular dynamics simulations, **CSM research day,** April 21 2023
84. Nakoa K. Webber, Ramandeep Kaur, and **Chun Wu**, Novel inhibitors to the Nsp15 protein of SARS-COV-2 identified by structure-based high-throughput Virtual screening with molecular dynamics simulations. **the symposium on translational research in infectious diseases**, the NJ Academic Drug Discovery Consortium, December 16, 2022, Kean University, Union, NJ 07083
85. Dylan Brunt, Justin Carbone and **Chun Wu,** Identifying Novel Nucleotide inhibitor Alternatives to Molnupiravir for Better Selectivity to RdRP of SARS-CoV-2 Using Structural Based Virtual Screening and Molecular Dynamic Simulations, **the symposium on translational research in infectious diseases**, the NJ Academic Drug Discovery Consortium, December 16, 2022, Kean University, Union, NJ 07083
86. Nicholas Paradis, Phillip M. Lakernick and **Chun Wu**, A random mutation model followed by SARS-CoV2 at both nucleotide and protein sequence observed in past 2 years, **the symposium on translational research in infectious diseases**, the NJ Academic Drug Discovery Consortium, December 16, 2022, Kean University, Union, NJ 07083
87. Lucas Bennett, Candice Bui-Linh, Nicholas J. Paradis, Hetanshi Choski, Jiancarlo Atienza, and **Chun Wu**, Novel Inhibitors to MmpL3 Transporter of Mycobacterium tuberculosis by Structure-Based High Throughput Virtual Screening and Molecular Dynamics Simulations, **the symposium on translational research in infectious diseases**, the NJ Academic Drug Discovery Consortium, **December 16,** 2022, Kean University, Union, NJ 07083
88. Dhrumi C. Patel, Katherine R Housman, Annie Tran, Phillip Lakernick, and **Chun Wu, Novel inhibitors to ADP Ribose Phosphatase of SARS-COV-2 identified by structure-based high-throughput virtual screening with molecular dynamics stimulations,** the NJ Academic Drug Discovery Consortium, December 16, 2022, Kean University, Union, NJ 07083
89. Justin Carbone and **Chun Wu**, Identifying Novel Inhibitors for Influenza A Polymerase Complex Refining Results for MD Simulation, **CSM research day, April 18 2022**
90. Mariya Hryb, Leah Davis, Stefi Lao, Nichole Daringer and **Chun Wu**, Structure and dynamics of HER2 directed Chimeric T-Cell Receptor (CAR) using homology modeling and all-atom molecular dynamics simulation with explicit solvent**, CSM research day, April 18 2022**

91. Alexandra Gerges, Gaelle Jean-Baptiste, Claudine M. Wrisley, Lauren Leung and **Chun Wu**, Identifying novel compounds similar to two FDA approved antagonist drugs to Calcitonin-Gene Related Peptide Receptor (CGRPR) using SwissSimiliary database search and Molecular Dynamics Simulations**, CSM research day, April 18 2022**
92. Lucas Bennett, Hetanshi Choksi, and **Chun Wu**, To identify Novel Inhibitors to MmpL3 transporter of Mycobacterium tuberculosis using Structure-based High Throughput Virtual Screening and Molecular Dynamics Simulations**, CSM research day, April 18 2022**
93. Nicholas J. Paradis, Phillip M. Lakernick and **Chun Wu**, A Random substitution Model Followed by SARS-COV-2 at Both the Nucleotide and Protein Sequence Level Observed in the Past 2 Years**, CSM research day, April 18 2022**
94. Daniel Mattera, Julia Gabriel, Elizabeth Uzhca, Erik Hoy and **Chun Wu**, Identifying Potential Inhibitors to 3-Chymotrypsin-like Protease (3CLpro) for Treating COVID-19 using structure-based virtual screening and molecular dynamics simulations**, CSM research day, April 18 2022**
95. Candice Bui-Linh, **Chun Wu**, Identifying Novel Anti-Cancer Inhibitors of the RAS-MAPK Pathway Using Virtual Screening and MD Simulation**, CSM research day, April 18 2022**
96. Nicholas Paradis, Phillip M. Lakernick and **Chun Wu**, A random mutation model followed by SARS-CoV2 at both nucleotide and protein sequence observed in past 2 years, **2021 MidAtlantic Bioinformatics Conference. November 8, 2021** *Trainee Poster Award Winner
97. Meeraj Amin and **Chun Wu** "The Analysis of the 5' Untranslated region mRNA Secondary Structure of SARS-COV-2 and its related genomic strains", **2021 MidAtlantic Bioinformatics Conference**. November 8, 2021
98. Mursalin Singh and **Chun Wu** "Was an Adenovirus Vaccine Challenge Trial Conducted on ICU patients at Wuhuan Jinyintan Hospital in Dec. 2019? Additional evidence to support Dr. Quay's finding." **2021 MidAtlantic Bioinformatics Conference**. November 8, 2021
99. M. Arba, N.J. Paradis, D. Brunt and **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 using AMBER compatible ligand force fields", **the ACS Fall 2021 National Meeting & Expo**, August 22-26, 2020.
100. V. Kumar, H.G. Liu and **C.Wu "**Drug repurposing against SARS-CoV-2 receptor binding domain using ensemble-based virtual screening and molecular dynamics simulations**" the ACS Fall 2021 National Meeting & Expo**, August 22-26, 2021.
101. Holli-Joi Sullivan, **Chun Wu***, Binding mechanism of CX-5461 to human telomeric, c-kit1 and c-Myc promoter G-quadruplexes, and a DNA duplex using free ligand molecular dynamics simulations, **ACS Spring 2020 National Meeting & Expo**, March 22-26, **2020**. (Converted into on-line poster, due to covid-19 pandemics)
102. Gilbert Fleischer, **Chun Wu*** Evaluation of Current Treatments and Identification of Novel Compounds Targetting the COVID 19 RNA-Dependent RNA Polymerase Using a Norovirus Homology Model, **Rowan University Student Scholars Symposium**, Glassboro, NJ, April 25-26, **2020** (Cancelled due to covid-19 pandemics)
103. Lucas F. Bennett, **Chun Wu*** Molecular modeling of MmpL3 inhibitor SQ109 and high-throughput virtual screening identifies potential therapeutic alternatives for Mycobacterium tuberculosis. **Rowan University Student Scholars Symposium**, Glassboro, NJ, April 25-26**, 2020** (Cancelled due to covid-19 pandemics)
104. Brian Chen, and **Chun Wu*** Probing the binding pathway of a disubstituted benzofuran compound (D089-0563) to c- MYC G-quadruplex using free ligand binding simulations and Markov State Model analysis, **Rowan University Student Scholars Symposium**, Glassboro, NJ, April 25-26, **2020** (Cancelled due to covid-19 pandemics)
105. Harika Aluwala, **Chun Wu*** Molecular modelling of PF-06882961 a novel small molecule agonist for GLP-1 receptor and high throughput virtual screening to identify novel compounds **Rowan University Student Scholars Symposium**, Glassboro, NJ, April 25-26, **2020** (Cancelled due to covid-19 pandemics)
106. Kirsten B. Hatchell, **Chun Wu*** Molecular modeling of selective inhibitor Erdafitinib to activating cancer mutations N540K and K650E in FGFR kinases and identifying novel inhibitor by high throughput virtual

screening, **Rowan University Student Scholars Symposium**, Glassboro, NJ, April 25-26, **2020** (Cancelled due to covid-19 pandemics)

107. Dylan J. Brunt, **Chun Wu*** Investigation of neuropeptide receptor subtype NPFF2 as a potential therapeutic target for small molecule peptide mimetics in the aid of nociception regulation and opioid modulation, **Rowan University Student Scholars Symposium**, Glassboro, NJ, April 25-26, **2020** (Cancelled due to covid-19 pandemics)

108. Emily Dean **Chun Wu*** Investigation of neuropeptide receptor subtype NPFF1 as a potential therapeutic target for small molecule peptide mimetics aiding in nociception regulation and opioid modulation, **Rowan University Student Scholars Symposium**, Glassboro, NJ, April 25-26, **2020** (Cancelled due to covid-19 pandemics)

109. Emily Dean, **Chun Wu***Probing the active conformation of the delta opioid receptor by an agonist ADL5859 using molecular dynamic simulation with explicit membrane, **Rowan University Student Scholars Symposium**, Glassboro, NJ, April 25-26, **2020** (Cancelled due to covid-19 pandemics)

110. Nicholas J. Paradis, **Chun Wu*** Probing the Binding Pathways of the Plant Alkaloid Chelerythrine to KRAS DNA G-Quadruplex via Free-Ligand Binding Simulations and Markov State Modeling Analyses, **Rowan University Student Scholars Symposium**, Glassboro, NJ, April 25-26, **2020** (Cancelled due to covid-19 pandemics)

111. Holli-Joi Sullivan, **Chun Wu*** Binding mechanism of CX-5461 to human telomeric, c-kit1 and c-Myc promoter G-quadruplexes, and a DNA duplex using free ligand molecular dynamics simulations, **Rowan University Student Scholars Symposium**, Glassboro, NJ, April 25-26, **2020** (Cancelled due to covid-19 pandemics)

112. Michael J. Pino, **Chun Wu*** Molecular Modeling of Helicase inhibitors of CoVID-19 virus and identifying novel inhibitors by high throughput virtual screening, **Rowan University Student Scholars Symposium, Glassboro**, NJ, April 25-26, **2020** (Cancelled due to covid-19 pandemics)

113. **Wu C**, TED_style talk, **CSM Research Expo** , May 3, **2019**

114. **Wu C**, My 20-year Journey in Using HPC for Scientific Research: Pitfalls and Tips. **Workshop on High-Performance Computing**, March 28, **2019**

115. Griffin Fountain, Subash Jonnalagadda, Claude Krummenacher and **Chun Wu***, High throughput virtual screening of ZINC drug-like ligand database against the second binding site Glycoprotein D (gD) of herpes simplex virus 1 toward a more potent inhibitor, **Rowan University Student Scholars Symposium**, Glassboro, NJ, April 25-26**, 2019**

116. Griffin Fountain, Simranjit Kaur, Claude Krummenacher and **Chun Wu**, Glycoprotein D of herpes simplex virus probed by all-atom molecular dynamics simulations, **Rowan University Student Scholars Symposium**, Glassboro, NJ, April 25-26, **2019**

117. Carina Olivas, Alexandre. Ilitchev, Maxwell J. Giammona, Sarah L. Cloud, Kristi L. Cantrell, Steven K. Buratto, Michael T. Bowers, **Chun Wu**, Hetero-oligomeric Amyloid Assembly and Mechanism: Prion Fragment PrP(106-126) Catalyzes the Islet Amyloid Polypeptide β-Hairpin, **Rowan University Student Scholars Symposium**, Glassboro, NJ, April 25-26, **2019**

118. Nicolas Scorese and **Chun Wu**, Binding of Peptide Agonist Urocortin, and Small Molecule Antagonist CP 376395 to the CRF1 Receptor Probed by Molecular Dynamics Simulations, **Rowan University Student Scholars Symposium**, Glassboro, NJ, April 25-26**, 2019**

119. Michael J. Pino Jr., Emily Dean, Charles Cooper, Thomas Keck and **Chun Wu**, Joint Computational-Experimental Drug Discovery of Novel Biased Agonists to Dopamine D2 Receptor toward Better Schizophrenia/Parkinson's Medications, **Rowan University Student Scholars Symposium**, Glassboro, NJ, April 25-26, **2019**

120. Jacqueline C. Mohen, John Jacobson, Dylan J. Brunt and **Chun Wu**, Molecular Dynamics Study of Intrinsic Activation of Four Night Blindness Mutations A292E, A295V, G90D, and T94I in Human GPCR Rhodopsin, **Rowan University Student Scholars Symposium**, Glassboro, NJ, April 25-26, **2019**

121. Nicolas Scorese and **Chun Wu**, GLP-1 Receptor in Complex with a Full Agonist and a Biased Agonist Probed by Molecular Dynamics Simulations, **Rowan University Student Scholars Symposium**, Glassboro, NJ, April 25-26, **2019**

122. Griffin Fountain and **Chun Wu**, Binding of a Disubstituted Benzofuran Derivative (DBD) to C-MYC promoter G-quadruplex using free ligand molecular dynamics simulations **Rowan University Student Scholars Symposium**, Glassboro, NJ, April 25-26, **2019**

123. Nikki D'Oliviera, Gregory A. Caputo, Timothy Vaden, and **Chun Wu**, The Computational Study of the Unfolding of Azurin at Melting Temperature (313K) in Ionic Liquid OMIMCl, **Rowan University Student Scholars Symposium**, Glassboro, NJ, April 25-26, **2019**

124. Joshua Freyer, Wen Liu, **Chun Wu**, Development of Small Molecule Inhibitors to Lysine-specific histone demethylase 1 (LSD1), Rowan University Student Scholars Symposium, Glassboro, NJ, April 25-26, **2019**

125. Siyan Liao, Emily Dean, Wen Liu, and **Chun Wu**, High Through-Put Virtual Screening on inhibitors binding PD-L1 or/and PD-L2 for cancer immuno-therapy, Rowan University Student Scholars Symposium, Glassboro, NJ, April 25-26, **2019**

126. Brian Chen, Norman Fultang, Bela Peethambaran, Subash Jonnalagadda, and **Chun Wu**, In-Silico Docking of Rx7, a novel ROR1-inhibitor that represses Triple Negative Breast Cancer survival, to ROR-1 using Homology Modeling and Active Site Mapping, Rowan University Student Scholars Symposium, Glassboro, NJ, April 25-26, **2019**

127. Lucas Bennett and **Chun Wu**, Binding of Selective Antagonist Istradefylline to Human Adenosine A2A Receptor Probed by Molecular Dynamics Simulations, Rowan University Student Scholars Symposium, Glassboro, NJ, April 25-26**, 2019**

128. Holli-Joi Sullivan and **Chun Wu**, Binding of BRACO19 to a Telomeric G-Quadruplex DNA Probed by All-Atom Molecular Dynamics Simulations with Explicit Solvent, Rowan University Student Scholars Symposium, Glassboro, NJ, April 25-26, **2019**

129. Holli-Joi Sullivan and **Chun Wu**, The Computational Study of Anti-Diabetic Agonist Chiglitazar with Human Peroxisome Proliferator-Activated Receptors, Rowan University Student Scholars Symposium, Glassboro, NJ, April 25-26, **2019**

130. Holli-Joi Sullivan and **Chun Wu**, Binding of CX-5461 to human telomeric, c-KIT1 and c-Myc promoter G-quadruplexes, and a DNA duplex using free ligand molecular dynamics simulations, Rowan University Student Scholars Symposium, Glassboro, NJ, April 25-26**, 2019**

131. Amy Erhard and **Chun Wu**, Comparison of antagonist and agonist molecular dynamics simulations of the δ–opioid receptor to verify conformational change from inactive to active states, Rowan University Student Scholars Symposium, Glassboro, NJ, April 25-26, **2019**

132. Siyan Liao, Himani Bhakta, Jia Song, Yanling Song, Chaoyong Yang and **Chun Wu**, Probing the Binding of a Quadruple-DNA to EpCAM using Docking and Molecular Dynamics Simulation, Rowan University Student Scholars Symposium, Glassboro, NJ, April 25-26, 2019

133. Stephen Ahwin, John Alviar, Micheal Pino, Marshall Asbury, and **Chun Wu**, Survey of GPCR Structures for Understanding Activation Mechanism & Virtual Screening, Rowan University Student Scholars Symposium, Glassboro, NJ, April 25-26, **2019**

134. Deirdra McNeil and **Chun Wu,** Investigation of Serotonin Receptor Allelic Variations In Modulating Efficacy of Selective Serotonin Reuptake Inhibitors Using Homology Modeling And Molecular Docking, Rowan University Student Scholars Symposium, Glassboro, NJ, April 25-26**, 2019**

135. SARAH HALIM, JONATHAN RESTREPO, and **Chun WU**, The Folding Pathway of RNA G-quadruplex Containing ALS-FTD Related G4C2 Repeat 85 Probed by Replica Exchange Molecular Dynamics Simulations with Explicit Solvent, Rowan University STEM symposium, Glassboro, NJ, April 20, **2018**

136. CECILIA G. FLOYD, and **Chun Wu**, Probing the Biased Agonism of TRV-130 on μ-opioid receptor (MOR) using Replica Exchange Molecular Dynamics (REMD) Simulations, Rowan University STEM symposium, Glassboro, NJ, April 20**, 2018**

137. ALEXANDRA N. CAMPBELL, and **Chun Wu**, The Binding Mode Pathways of Chelerythrine with 2F8U, 5I2V, and 2M27 G-quadruplexes using Molecular Dynamics Simulations, Rowan University STEM symposium, Glassboro, NJ, April 20, **2018**

138. SHAINA NOGLE, Xiaoyan Wang, and **Chun Wu,** The Computational Study of Anti-Diabetic Agonist Chiglitazar with Human Peroxisome Proliferator Activated Receptors Using Docking and Molecular Dynamics Simulations, Rowan University STEM symposium, Glassboro, NJ, April 20, **2018**
139. ASHLEIGH M. MCCONNELL, and **Chun Wu,** Binding of Beta-Arrestin Biased Ligands (Isoetharine and Carvelilol) and an Unbiased Ligand (Isoproterenol) to Beta2-Adrogenic Receptor Using Molecular Dynamics Simulations, Rowan University STEM symposium, Glassboro, NJ, April 20, **2018**
140. NICOLAS A. SCORESE, and **Chun Wu**, Binding of Peptide Agonist Urocortin, Peptide Antagonist Astressin, and Small Molecule Antagonist CP 154,526 to the CRF1 Receptor Probed by Molecular Dynamics Simulations, Rowan University STEM symposium, Glassboro, NJ, April 20, **2018**
141. HOLLI-JOI SULLIVAN, and **Chun Wu**, Binding of CX-5461 to Human Telomeric, c-kit1 and cMyc Promoter G-quadruplexes, and a DNA Duplex Using Free Ligand Molecular Dynamics Simulations, Rowan University STEM symposium, Glassboro, NJ, April 20, **2018**
142. HANNAH M. HOAG, SAFAA SADER, and **Chun Wu**, In Silico Visioning Communications between Signal Ligands on Beta2 Adrenergic Receptor and Effecter Guanine Nucleotide (GDP) on G-Protein Using Molecular Dynamics simulations in explicit membrane, Glassboro, NJ, April 20, **2018**
143. MIRANDA K. PREZIOSI, and **Chun Wu,** Binding of Bethanechol (agonist) and QNB (antagonist) to human M2 muscarinic acetylcholine receptor probed by molecular dynamics simulations with explicit membrane, Rowan University STEM symposium, Glassboro, NJ, April 20, **2018**
144. NAZRA A. SYED, and **Chun Wu**, To Decipher the Activation Mechanism of an Atypical Antidepressant Drug, Tianeptine, Using Docking and Molecular Dynamics Simulations with Explicit Membrane, Rowan University STEM symposium, Glassboro, NJ, April 20**, 2018**
145. JOSE B. PARRA, and **Chun Wu,** To Probe the Binding of Gambogic Acid and Plerixafor, an Anti-Cancer Drug, to CXCR4 Using Molecular Dynamics Simulation with Explicit Membrane, Rowan University STEM symposium, Glassboro, NJ, April 20**, 2018**
146. DAEGUN A. BONG, and **Chun Wu,** To Probe the Working Mechanism of ML380, a Positive Allosteric Modulator, and ML375, a Negative Allosteric Modulator of the M5 Muscarinic Acetylcholine Receptor Using Molecular Dynamics Simulations, Rowan University STEM symposium, Glassboro, NJ, April 20**, 2018**
147. JOHN J. VIZZINI, and **Chun Wu,** Binding of MM41 to the Promoter G-quadruplex of Oncogenes BCL-2 and K-RAS Using Free Ligand Binding Molecular Dynamics Simulations, Rowan University STEM symposium, Glassboro, NJ, April 20, **2018**
148. JUN CAI, and **Chun Wu,** Homology Modeling of Human vegrf-2 Promoter Gquadruplex and Its Binding with EMICORON Probed by Free Ligand Binding Molecular Dynamics Simulations, Rowan University STEM symposium, Glassboro, NJ, April 20**, 2018**
149. GRIFFIN M. FOUNTAIN, and **Chun Wu**, Binding of a Disubstituted Benzofuran Derivative (DBD) to C-MYC promoter G-quadruplex using free ligand molecular dynamics simulations, Rowan University STEM symposium, Glassboro, NJ, April 20, **2018**
150. **Wu C** Montgomery DW "Molecular Dynamics Simulation of Biased Agonists at the Dopamine D2 Receptor Suggests the Mechanism of Receptor Functional Selectivity**" the 255th ACS National Meeting**, New Orleans, LA, March 18-22, **2018**
151. Mohen J, **Wu C** *"Shedding light on the conformational changes leading to intrinsic activation of four night blindness mutations G90D, T94I, A292E, A295V on the human GPCR rhodopsin: A molecular dynamics simulation study",* the 254th ACS National Meeting in Washington, DC, August 20-24, 2017
152. Radicella C, Fasano T, Persad V, **Wu C** *"Binding at the telomeric G-quadruplex-duplex interface: A computational study"*, the 254th ACS National Meeting in Washington, DC, August 20-24, 2017
153. Griffin Fountain and **Chun Wu**, *"Binding of a Disubstituted Benzo furan Derivative (DBD) to C-MYC promoter G-quadruplex using free ligand molecular dynamics simulations "* Chemistry Fall Research Symposium, November 16, 2018, Science Hall Atrium/Planetarium
154. Holli-Joi Sullivan and **Chun Wu**, *"Binding of CX-5461 to human telomeric, c-KIT1 and c-Myc promoter G-quadruplexes, and a DNA duplex using free ligand molecular dynamics simulations"* Chemistry Fall Research Symposium, November 16, 2018, Science Hall Atrium/Planetarium

155. Floyd CG, **Wu C** *"Probing Biased Activation of μ-opioid Receptor by the Biased Agonist PZM21 Using all Atom Molecular Dynamic Simulation",* Science, Technology, Engineering, Mathematics (STEM) Undergraduate Research Symposium at Rowan University, Glassboro, NJ, April 21, 2017
156. Montgomery DW, **Wu C** *"Molecular Dynamics of Biased Agonists at the Dopamine D2 Receptor Suggests the Mechanism of Receptor Functional Selectivity",* Science, Technology, Engineering, Mathematics (STEM) Undergraduate Research Symposium at Rowan University, Glassboro, NJ, April 21, 2017
157. McConnell AM, **Wu C** *"Probing the active conformation of the delta opioid receptor by multiple agonists using molecular dynamic simulation with explicit membrane",* Science, Technology, Engineering, Mathematics (STEM) Undergraduate Research Symposium at Rowan University, Glassboro, NJ, April 21, 2017
158. Mohen J, **Wu C** *"Shedding Light on the Conformational Changes Leading to Intrinsic Activation of Four Night Blindness Mutations G90D, T94I, A292E, A295V on the Human GPCR Rhodopsin: A Molecular Dynamics Simulation Study",* Science, Technology, Engineering, Mathematics (STEM) Undergraduate Research Symposium at Rowan University, Glassboro, NJ, April 21, 2017
159. Readmond C, **Wu C** *"Investigating detailed interactions between novel PAR1 antagonist F16357 and the receptor using docking and molecular dynamic simulations",* Science, Technology, Engineering, Mathematics (STEM) Undergraduate Research Symposium at Rowan University, Glassboro, NJ, April 21, 2017
160. Sullivan HJ, Nogle S, **Wu C** *"Determining the Source of Carfentanil's Potency Using Molecular Dynamic Simulation for Pharmaceutical Development",* Science, Technology, Engineering, Mathematics (STEM) Undergraduate Research Symposium at Rowan University, Glassboro, NJ, April 21, 2017
161. Radicella CS, **Wu C** *"Binding at the Telomeric G-quadruplex-Duplex Interface",* Science, Technology, Engineering, Mathematics (STEM) Undergraduate Research Symposium at Rowan University, Glassboro, NJ, April 21, 2017
162. Radicella CS, **Wu C** *"Non-peptide Agonist and Antagonist Binding to the Oxytocin Receptor",* Science, Technology, Engineering, Mathematics (STEM) Undergraduate Research Symposium at Rowan University, Glassboro, NJ, April 21, 2017
163. Machireddy B, Jonnalagadda SC, Ramanujachary KV, **Wu C** *"Computer Aided Drug Design in Boron Therapeutics targeting Onychomycosis",* Science, Technology, Engineering, Mathematics (STEM) Undergraduate Research Symposium at Rowan University, Glassboro, NJ, April 21, 2017
164. Machireddy B, Kalra G, Jonnalagadda SC, Ramanujachary KV, **Wu C** *"Probing the Binding mechanism of BRACO19 to Parallel Quadruplexes from Human Telomeric DNA using Molecular Dynamics Simulation with a Free Ligand",* Science, Technology, Engineering, Mathematics (STEM) Undergraduate Research Symposium at Rowan University, Glassboro, NJ, April 21, 2017
165. Ge L, Moran-Nesteor JL, **Wu C** *"Binding of Agonist and Antagonist to Human P2Y12 Receptor Using Molecular Dynamics Simulation: Probe Rceptor Activation Mechanism",* Science, Technology, Engineering, Mathematics (STEM) Undergraduate Research Symposium at Rowan University, Glassboro, NJ, April 21, 2017
166. Bong DA, Perhach JE, **Wu C** *"Recognition Mechanisms of Muscarinic Acetylcholine Receptors M1-5 by Subtype Selective Agonists and Antagonists",* Science, Technology, Engineering, Mathematics (STEM) Undergraduate Research Symposium at Rowan University, Glassboro, NJ, April 21, 2017
167. Sader S, **Wu C** *"In silico Visioning of G Protein-GDP Complex Communications with GPCR Bound to Different Ligands Using Molecular Dynamic Simulations in Explicit Membrane",* Science, Technology, Engineering, Mathematics (STEM) Undergraduate Research Symposium at Rowan University, Glassboro, NJ, April 21, 2017
168. Haila GJ, Krummenacher C, **Wu C** *"Novel approach to prevent herpes infection",* Science, Technology, Engineering, Mathematics (STEM) Undergraduate Research Symposium at Rowan University, Glassboro, NJ, April 21, 2017

169. Fountain GM, **Wu C** *"Predict Na+-sensitivity of A412997, an agonist to dopamine D4 receptor",* Science, Technology, Engineering, Mathematics (STEM) Undergraduate Research Symposium at Rowan University, Glassboro, NJ, April 22, 2017
170. Borrell KL, Stinger B, Cangclin C, DeFrates K, Caputo GA, **Wu C**, Vaden TD, " An Experimental & Molecular Dynamics Study of Red Fluorescent Protein mCherry in Novel Aqueous Amino Acid Ionic Liquids", Science, Technology, Engineering, Mathematics (STEM) Undergraduate Research Symposium at Rowan University, Glassboro, NJ, April 22, 2017
171. Hoag HM, Delesky EM, Mcallister SR, Fountain GM, **Wu C**, Keck TM, *"Development of binding of novel D4 receptor-selective compounds as agonists used to study neuropsychiatric disorders"*, Science, Technology, Engineering, Mathematics (STEM) Undergraduate Research Symposium at Rowan University, Glassboro, NJ, April 22, 2017
172. Crouch M, **Wu C** *"Analysis of Highly Selective/Functionally Selective Dopamine D3 Hybrid Ligand",* Science, Technology, Engineering, Mathematics (STEM) Undergraduate Research Symposium at Rowan University, Glassboro, NJ, April 21, 2016,
173. Crouch M, **Wu C** *"Analysis of Highly Selective/Functionally Selective Dopamine D3 Hybrid Ligand",* 7th Annual SJACS Undergraduate Research Symposium, Glassboro, NJ, April 23, 2016
174. Tan K, Smith A, **Wu C** *"Molecular Simulation Comparison of TRV-130 and Morphine: Understanding Biased Agonism at the mu-Opioid Receptor",* Science, Technology, Engineering, Mathematics (STEM) Undergraduate Research Symposium at Rowan University, Glassboro, NJ, April 21, 2016,
175. Tan K, Smith A, **Wu C** *"Molecular Simulation Comparison of TRV-130 and Morphine: Understanding Biased Agonism at the mu-Opioid Receptor",* 7th Annual SJACS Undergraduate Research Symposium, Glassboro, NJ, April 23, 2016
176. Muller ACG**, Wu C** *"Binding of Fexofenadine to Human, Dog and Cat Histamine H1 Receptor",* Science, Technology, Engineering, Mathematics (STEM) Undergraduate Research Symposium at Rowan University, Glassboro, NJ, April 21, 2016,
177. Muller ACG, Wu C "Binding of Fexofenadine to Human, Dog and Cat Histamine H1 Receptor",7th Annual SJACS Undergraduate Research Symposium, Glassboro, NJ, April 23, 2016
178. Berry KM**, Wu C** *"A Mechanism Study on Osimertinib, a Third Generation Epidermal Growth Factor Receptor Tyrosine Kinase Inhibitor Drug Using Covalent/Non-Covalent Docking and All-Atom Molecular Dynamics Simulation",* Science, Technology, Engineering, Mathematics (STEM) Undergraduate Research Symposium at Rowan University, Glassboro, NJ, April 21, 2016
179. Deleon C**, Wu C** *"Why EPPTB, a Good Antagonist to Mouse TAAR1 Receptor, Does Not Work Well on Human TAAR1?",* Science, Technology, Engineering, Mathematics (STEM) Undergraduate Research Symposium at Rowan University, Glassboro, NJ, April 21, 2016,
180. Deleon C**, Wu C** *"Why EPPTB, a Good Antagonist to Mouse TAAR1 Receptor, Does Not Work Well on Human TAAR1?",* 7th Annual SJACS Undergraduate Research Symposium, Glassboro, NJ, April 23, 2016
181. Meremianin A**, Wu C** *"Binding of the Anti-Tumor Drug Trabectedin to DNA Target, Probed by All-Atom Molecular Dynamics Simulation",* Science, Technology, Engineering, Mathematics (STEM) Undergraduate Research Symposium at Rowan University, Glassboro, NJ, April 21, 2016,
182. Meremianin A, Wu C "Binding of the Anti-Tumor Drug Trabectedin to DNA Target, Probed by All-Atom Molecular Dynamics Simulation", 7th Annual SJACS Undergraduate Research Symposium, Glassboro, NJ, April 23, 2016
183. Maurer J, **Wu C** *"Biased Agonism of TRV027 to Angiotensin Type 1 Receptor Probed by All-Atom Molecular Dynamics Analysis with an Explicit Membrane",* Science, Technology, Engineering, Mathematics (STEM) Undergraduate Research Symposium at Rowan University, Glassboro, NJ, April 21, 2016,
184. Maurer J, **Wu C** *"Biased Agonism of TRV027 to Angiotensin Type 1 Receptor Probed by All-Atom Molecular Dynamics Analysis with an Explicit Membrane",* 7th Annual SJACS Undergraduate Research Symposium, Glassboro, NJ, April 23, 2016
185. Sader S**, Wu C** *"Structural and Dynamic Analysis of Wild and Splice Variants Opioid Receptors by Homology Modeling, Docking and All Atoms Molecular Dynamic Simulation with Explicit Membrane",*

Science, Technology, Engineering, Mathematics (STEM) Undergraduate Research Symposium at Rowan University, Glassboro, NJ, April 21, 2016,

186. Chea J, **Wu C** *"Working Mechanism of Negative Allosteric Modulators MFZ 10-7, MTEP and Fenobam Docked to Metabotropic Glutamate Receptor 5 (mGluR5) and Probed by All-Atom Molecular Dynamics Simulations of Docked Complexes with Explicit Membrane",* Science, Technology, Engineering, Mathematics (STEM) Undergraduate Research Symposium at Rowan University, Glassboro, NJ, April 21, 2016,

187. Chea J, **Wu C** *"Working Mechanism of Negative Allosteric Modulators MFZ 10-7, MTEP and Fenobam Docked to Metabotropic Glutamate Receptor 5 (mGluR5) and Probed by All-Atom Molecular Dynamics Simulations of Docked Complexes with Explicit Membrane",* 7th Annual SJACS Undergraduate Research Symposium, Glassboro, NJ, April 23, 2016

188. Kalra G**, Wu C** *"Binding Challenge For Bevirimat , A HIV Maturation Inhibitor, To Its Protein Target" Probed By All-Atom Molecular Dynamics Simulation With Explicit Solvent",* Science, Technology, Engineering, Mathematics (STEM) Undergraduate Research Symposium at Rowan University, Glassboro, NJ, April 21, 2016,

189. Kalra G**, Wu C** *"Binding Challenge For Bevirimat , A HIV Maturation Inhibitor, To Its Protein Target"* 7th Annual SJACS Undergraduate Research Symposium, Glassboro, NJ, April 23, 2016

190. Pagnoncelli IB**, Wu C** *"Activation Mechanism of Delta Opioid Receptor, Probed by All-Atom Molecular Dynamics Simulation of 11 Common Agonist/Antagonists with the Receptor in Explicit Membrane",* Science, Technology, Engineering, Mathematics (STEM) Undergraduate Research Symposium at Rowan University, Glassboro, NJ, April 21, 2016, 7th Annual SJACS Undergraduate Research Symposium, Glassboro, NJ, April 23, 2016

191. Fisher P, Floyd CG, McConnell AM, **Wu C** *"Virtual Screening of Ligands Targeting 6TM Splice Variants of Mu-Opioid Receptors: To Identify Novel Analgesics Comparable to IBNtxA",* Science, Technology, Engineering, Mathematics (STEM) Undergraduate Research Symposium at Rowan University, Glassboro, NJ, April 21, 2016,

192. Fisher P, Floyd CG, McConnell AM, **Wu C** *"Virtual Screening of Ligands Targeting 6TM Splice Variants of Mu-Opioid Receptors: To Identify Novel Analgesics Comparable to IBNtxA",*11th Annual Undergraduate Research Symposium at William Paterson University, Wayne, JJ, April 9, 2016

193. Fisher P, Floyd CG, McConnell AM, **Wu C** "Virtual Screening of Ligands Targeting 6TM Splice Variants of Mu-Opioid Receptors: To Identify Novel Analgesics Comparable to IBNtxA", 7th Annual SJACS Undergraduate Research Symposium, Glassboro, NJ, April 23, 2016

194. Mullholland KA**, Wu C** *"A Mechanical Study of Topisomerase I Mutations Leading to Anti-Cancer Drug Resistance in Camptothecin Analogs and Lucanthone",* Science, Technology, Engineering, Mathematics (STEM) Undergraduate Research Symposium at Rowan University, Glassboro, NJ, April 21, 2016,

195. Mullholland KA, **Wu C** "A Mechanical Study of Topisomerase I Mutations Leading to Anti-Cancer Drug Resistance in Camptothecin Analogs and Lucanthone", 7th Annual SJACS Undergraduate Research Symposium, Glassboro, NJ, April 23, 2016

196. Mullholland KA**, Wu C** *"Binding Analysis of Telomestatin to a Telomeric G-Quadruplex DNA Probed by All-Atom Molecular Dynamics Simulations",* Science, Technology, Engineering, Mathematics (STEM) Undergraduate Research Symposium at Rowan University, Glassboro, NJ, April 21, 2016,

197. Mullholland KA, **Wu C** "*Binding Analysis of Telomestatin to a Telomeric G-Quadruplex DNA Probed by All-Atom Molecular Dynamics Simulations*", 7th Annual SJACS Undergraduate Research Symposium, Glassboro, NJ, April 23, 2016

198. Oliverira FSR, Wang XY, **Wu C** *"Activation Mechanism of Partial and Full Agonists to Peroxisome Proliferator-Activated Receptors, Probed by All-Atom Dynamics Simulation with Explicit Solvent",* Science, Technology, Engineering, Mathematics (STEM) Undergraduate Research Symposium at Rowan University, Glassboro, NJ, April 21, 2016,

199. Oliverira FSR, Wang XY**, Wu C** "*Activation Mechanism of Partial and Full Agonists to Peroxisome Proliferator-Activated Receptors, Probed by All-Atom Dynamics Simulation with Explicit Solvent*", 7th Annual SJACS Undergraduate Research Symposium, Glassboro, NJ, April 23, 2016

200. Yamabushi AM**, Wu C** *"Working mechanism of Nebivolol (antagonist), Pindolol (partial agonist) and Isoprenaline (agonist) to beta-1 adrenoreceptor, probed by homology modeling, docking and all-atom molecular dynamics simulation with explicit membrane",* Science, Technology, Engineering, Mathematics (STEM) Undergraduate Research Symposium at Rowan University, Glassboro, NJ, April 21, 2016
201. Kalra G, Maurer J, **Wu C** *"Binding Of BRACCO19 To A Telomeric Quadruplex, Probed By All-Atom Molecular Dynamics Simulation With Explicit Solvent",* Science, Technology, Engineering, Mathematics (STEM) Undergraduate Research Symposium at Rowan University, Glassboro, NJ, April 21, 2016,
202. Kalra G, Maurer J, **Wu C** *"Binding Of BRACCO19 To A Telomeric Quadruplex, Probed By All-Atom Molecular Dynamics Simulation With Explicit Solvent"* 7th Annual SJACS Undergraduate Research Symposium, Glassboro, NJ, April 23, 2016
203. Tenn AK**, Wu C** *"Working mechanism of propranolol (antagonist), salbutamol (partial agonist) and Isoprenaline (agonist) to beta-2 adrenoreceptor, probed by docking and all-atom molecular dynamics simulation with explicit membrane",* Science, Technology, Engineering, Mathematics (STEM) Undergraduate Research Symposium at Rowan University, Glassboro, NJ, April 21, 2016
204. Cai J, **Wu C** *"Working mechanism of agonists of (Compound-26 and Way-267464) and antagonist (DORA-39) binding to orexin receptor 2, probed by all-atom molecular dynamics simulations of the receptor-ligand complex with explicit membrane.",* Science, Technology, Engineering, Mathematics (STEM) Undergraduate Research Symposium at Rowan University, Glassboro, NJ, April 21, 2016
205. Siddiquei F, **Wu C** *"Binding of TMPyP4, a G-quadruplex ligand, to promoter of oncogenes c-Kit and Bcl-2 probed by all-atom molecular dynamics simulations",* Science, Technology, Engineering, Mathematics (STEM) Undergraduate Research Symposium at Rowan University, Glassboro, NJ, April 21, 2016
206. Syed N, **Wu C** "Activation mechanism of thyroid hormone alpha receptor by an agonist synthroid, probed by all-atom molecular dynamics simulations" Science, Technology, Engineering, Mathematics (STEM) Undergraduate Research Symposium at Rowan University, Glassboro, NJ, April 21, 2016
207. Fountain G, **Wu C** *"Interactions of agonist A412997 and antagonist A381393 with Dopamine D4 receptor probed by all-atom molecular dynamics simulations with explicit membrane",* Science, Technology, Engineering, Mathematics (STEM) Undergraduate Research Symposium at Rowan University, Glassboro, NJ, April 21, 2016
208. Fountain G, **Wu C** *"Interactions of agonist A412997 and antagonist A381393 with Dopamine D4 receptor probed by all-atom molecular dynamics simulations with explicit membrane",* 7th Annual SJACS Undergraduate Research Symposium, Glassboro, NJ, April 23, 2016
209. Hermandez JJS**, Wu C** *"Rolapitant as an antagonist of NK-1 receptor",* Science, Technology, Engineering, Mathematics (STEM) Undergraduate Research Symposium at Rowan University, Glassboro, NJ, April 21, 2016
210. Keck TM, **Wu C**, Fountina GM, Tkaczynski JA, Freund, JR, Bonizfazi A, Elleb erger M, Newman AH, Boateng CA Wu C, *"A rational drug design strategy for novel dopamine D4 receptor agonists",* Behavior, Biology and Chemistry: Translational Research in Addiction, San Antonio, TX, March 5-6, 2016
211. Kumar A, **Wu C *"****Binding of Analgesic Drugs to Their Targets (μ-Opioid Receptors) probed by Molecular Modeling****",*** Science, Technology, Engineering, Mathematics (STEM) Undergraduate Research Symposium at Rowan University, Glassboro, NJ, April 24, 2015
212. Mullholland K, **Wu C**, Shen ZH, Zheng YJ, *"Binding of Anti-cancer Ligands to Key G-Quadruplex DNA Structures probed by Molecular Dynamics Simulations"* Science, Technology, Engineering, Mathematics (STEM) Undergraduate Research Symposium at Rowan University, Glassboro, NJ, April 24, 2015

LIST OF INVITED TALKS PRIOR TO JOINING ROWAN

213. **Wu C** *"Molecular dynamics (MD) simulations: a powerful tool for biomedical research"*, East China Normal University, Shanghai, P. R. China, June, 2013
214. **Wu C** *"Molecular dynamics (MD) simulations: a powerful tool for biomedical research"*, Xiamen University, Xiamen, P. R. China, June, 2013

215. **Wu C** *"Molecular dynamics (MD) simulations: a powerful tool for biomedical research"*, Shangdong University, Jinan, P. R. China, June, 2013

216. **Wu C** *"Molecular dynamics (MD) simulations: a powerful tool for biomedical research"*, Fudan University, Shanghai, P. R. China, June, 2013

217. **Wu C** & Shea JE "*Structural basis for physiological and pathological activities of Islet Amyloid Polypeptide (IAPP) probed by molecular dynamics simulations*", 6th Worldwide Chinese Theoretical and Computational Chemistry Conference, Taipei, Taiwan, June. 2013

218. **Wu C** "*Molecular dynamics (MD) simulations: a powerful tool for biomedical research*", Stanford University, Palo Alto, CA, March, 2013

219. **Wu C** Dupuis NF, Bowers MT and Shea JE "*Folding and dimerization of type 2 diabetes amyloid forming amylin peptide using molecular dynamics simulations: potential drug targets*", The 11th National Conference of Quantum Chemistry, Hefei, China, May. 2011

220. **Wu C** "*Development of AMBER protein force fields and bio-applications of all-atom molecular dynamics simulations*", Shanghai Institute of Materia Medica, Chinese Academy of Sciences , Shanghai, China, May. 2011

221. **Wu C** "*Development of AMBER protein force fields and bio-applications of all-atom molecular dynamics simulations*", Fudan University, Shanghai, China, May. 2011

222. **Wu C** "*Computational modeling (sequence-structure-dynamics): a great opportunity for China*", Beijing Institute of Genomics, Chinese Academy of Science, Beijing, China, May. 2011

223. **Wu C** "*Development of AMBER protein force fields and bio-applications of all-atom molecular dynamics simulations*", College of Chemistry and Chemical Engineering, Graduate University of Chinese Academy of Science, Beijing, China, May. 2011

224. **Wu C** "*Molecular dynamics (MD) simulations: a great opportunity for China*", Xiamen University, Xiamen, China, May. 2011

225. **Wu C** *"Development of AMBER protein force fields and bio-applications of all-atom molecular dynamics simulations"*, Hong Kong University of Science & Technology, Hong Kong, China, May. 2011

226. **Wu C** "*Probing and optimizing functional small molecules and bio-molecules by molecular dynamics (MD) simulations*", LSU, LA, Feb. 2011

227. **Wu C** "*Dye binding, folding and aggregation of amyloid peptides probed by all-atom molecular dynamics (MD) simulations* ", LSU, LA, Feb. 2011

228. **Wu C,** M Grabenauer, Bowers MT & Shea JE "*Predicting structures of small non-amyloid and amyloid proteins using molecular dynamics simulation in implicit water*", Isolated Biomolecules and Biomolecular Interactions 2010, Berlin, Jun. 2010

229. **Wu C,** Shea JE& Bowers MT "*The Binding of Thioflavin-T and its Neutral Analog PIB to Cross-b-subunit of the Alzheimer Aβ9-40 peptide probed by Molecular Dynamics simulations*", College of Chemistry and Chemical Engineering, Graduate University of Chinese Academy of Science, Beijing, China, Dec. 2009

230. **Wu C** "*Molecular dynamics simulations and applications*", Xiamen University, Xiamen, China, Dec. 2009

231. **Wu C** & Shea JE "*ab initio folding of α/β protein by All-atom Molecular Dynamics*", 2nd ITP international symposium, Santa Barbara, USA, Nov. 2009

232. **Wu C,** Shea JE& Bowers MT "*An introduction to protein and peptide aggregation*", 238th American Chemical Society National Meeting & Exposition, Washington, DC, USA, Aug. 2009

233. **Wu C,** Shea JE& Bowers MT "*Multiple binding sites of Alzheimer's $A\beta_{16-22}$ protofibril-oligomer by Thioflavin-T and its neutral analog (BTA-1) observed in molecular dynamics simulations*", College of Chemistry and Chemical Engineering, Graduate University of Chinese Academy of Science, Beijing, China, Feb. 2008

234. ZG LIN, **C. WU**, YB ZHAO, YG TONG, JG XU, SK YANG, " Applying accumulation method to tridimensional fluorescence spectrometry" Proceeding of the 5th China Luminescence Spectroscopy Analysis Conference, P36-37(1996)

235. ZG LIN, YG TONG, **C. WU**, XP XIAO, YB ZHAO, JG XU, "Obtainment of any type of synchronous fluorescence spectra of two components by computational method" Proceeding of the 5th China Luminescence Spectroscopy Analysis Conference, P34-35(1996)

236. ZG LIN, YG TONG, **C. WU,** XP XIAO, YB ZHAO, JG XU "Quick obtainment of excitation emission matrix (EEM) of multi-component by linear addition of the EEM of each component " Proceeding of the 5th China Luminescence Spectroscopy Analysis Conference P32-33(1996)

237. ZG LIN, **C. WU**, YG TONG, YB ZHAO, JG XU, SK YANG, "Quick obtainment of excitation emission matrix(EEM) of single component from its excitation and emission spectra of fluorescence by numerical orthogonal computing method", Proceeding of the 5th China Luminescence Spectroscopy Analysis Conference P31-32, (1996)

CURRENT RSEARCH SCHOLARS AND STUDENTS IN THE LAB

Women, persons with disabilities, and three racial and ethnic groups—blacks, Hispanics, and American Indians or Alaska Natives—are underrepresented in science and engineering.

No.	Name	Term	Project	After graduation
	Postdoc			
	Graduate students			
34	Nicholas Paradis (PhD, Pharm Sci)	09/2022-present	G-quadruplex, Ionic Liquid	
33	Khushi Jain	09/2023-present	Ev69	
32	Hetanshi Choksi	09/2023-present	Monkeypox	
31	Drashti Gedia	09/2022-05/2024	Anti-cancer	
30	Nishtha Patel	09/2022-05/2024	Anti-cancer	
29	Mariya Hryb (MS, Pharm Sci)	01/2022-01/2024	CAR-T	
28	Justin David Carbone (MS, Pharm Sci)	09/2022-05/2024	COVID-19	
27	Annie Tran (MS, Pharm Sci)	09/2022-05/2024	COVID-19	
26	Ramandeep Kaur (MS Bioinfo)	09/2022-05/2024	COVID-19	
	Undergraduate students			
120	Priyaben Patel	09/2024-present	Virus evolution	
119	Thao My Nguyen	01/2024-present	Virus evolution	
118	Samee Ahsan Khan	09/2023-present	Ebola	Applying for Medical School
117	Lisette Sotelo-Flores	01/2024-present	Virus evolution	
116	Gianna Christina Thwaites	01/2024-present	Virus evolution	Applying for Medical School

PAST RSEARCH SCHOLARS AND STUDENTS IN THE LAB

No.	Name	Term	Project	After graduation
	Visiting professor/Postdoc			
05	Dr. Abdullahi Ibrahim Uba	11/2019-01/2023	GPCR receptor	Assistant Professor Position Dept Mol Biol and Gen, Istanbul AREL University, Istanbul, Turkey
04	Prof. Kai Tan	03/2015-03/2016	Pain/opioid receptor	Collaboration

03	Prof. Xiaoyan Wang	07/2015-01/2016	Diabetes/ PPAR	Collaboration
02	Prof. Liao Siyan	09/2018-01/2021	GPCR receptor	Collaboration
01	Dr. Vikash Kumar	08/2019-08/2021	GPCR receptor	Postdoc position
	Graduate students			
25	Nicholas Paradis (PhD, Pharm Sci)	09/2020-05/2022	G-quadruplex, Ionic Liquid	PhD in Pharm Sci Rowan University
24	Philip Lakernick (MS, Pharm Sci)	09/2019-05/2022	COVID-19	Navy
23	Dylan Brunt (MS, Pharm Sci)	09/2019-05/2021	GPCR receptor	Scientist at Tris Pharma
22	Emily Dean (MS, Pharm Sci)	09/2019-05/2021	GPCR receptor	Data Analyst Local Company
21	Lucas Bennett (MS, Pharm Sci)	09/2019-05/2021	gD	Local School
20	Michael Pino (MS, Pharm Sci)	09/2019-05/2021	GPCR receptor	Local Company
19	Harika Aluwala (MS, Pharm Sci)	09/2019-05/2021	GPCR receptor	Research Associate at Charles River Laboratories
18	Dhrumiben Patel (MS, Bioinformatics)	09/2020-2021	COVID-19	Scientist III Sanofi
17	Nakoa Webber (MS, Pharm Sci)	09/2020-2021	COVID-19	PhD program, Drexel University, College of Medicine
16	Brian Chen (MS, Bioinfo)	09/2018-05/2020	MSM	Software engineer Illumina
15	Holli Sullivan (MS, Pharm Sci)	09/2018-05/2020	G-quadruplex	PhD in pharmaceutical Science at UNC Chapel Hill
14	Amy Erhard (MS, Bioinfo)	09/2018-01/2020	GPCR receptor	Data Analyst Local Company
13	Hannah Hoag (MS, Pharm Sci)	05/2017-05/2018	Dopamine D4 receptor/mGluR5/G-protein	PHD, Biochemsitry, Thomas jefferson University
12	Griffin Fountain (MS, Pharm Sci)	09/2017-05/2019	Dopamine D4 receptor/D3	Rowan, Chemical Engineering (MS) PhD in Pharmaceutical Sciences, Virginia Commonwealth University
	Nicolas Scorese (MS, Bioinformatics)	09/2017-05/2019	OTR receptor	PDS Life Sciences,
11	Daegun Bong (MS, Bioinformatics)	01/2017-05/2018	M3 receptor, PPAR	Data Analyst PDS Life Sciences

10	Jun Cai (MS, Pharm Sci)	01/2016-05/2018	PPAR receptors	PhD program, George State University
09	Babitha Machireddy(MS, Pharm Sci)	05/2016-09/2017	BRACO19	PhD in chemistry, University of Arkansas
08	Jacquelin Mohen (MS, Pharm Sci)	01/2017-05/2017	Rhodopsin	Pharmacy Technician, CSV Health
07	Kenneth M Berry (MS, Bioinformatics)	01/2016-08/2016	Tyrosine Kinase Inhibitor	Local Company
06	Kelly Mulholland (MS, Bioinformatics)	02/2015-05/2016	Cancer/Top1/REMD	PhD program in Univ. of Delaware Postdoc Upenn Senior Scientist AstraZeneca
05	Safaa Sader (MS, Pharm Sci)	07/2015-05/2016	Pain/opioid receptor	PhD program in Auburn Univ.
04	Nicolas Scorese (MS, Bioinformatics)	09/2017-05/2019	OTR receptor	Data Analyst, PDS life science
	Undergraduate students			
115	St Pierre, Hunter (BS, Bioinfo)	01/2023-05/2023	Anti-cancer	
114	Alicia Petrany (BS, Bioinfo)	01/2023-05/2023	Anti-cancer	
113	Jasmine Mott (BS, Biochem)	01/2023-05/2023	COVID-19	Temple University Kornberg School of Dentistry
112	Amber Mott (BS, Biochem)	01/2023-05/2023	COVID-19	Temple University Kornberg School of Dentistry
111	Americus Novaly Palillero (BS, Biochem)	01/2023-09/2023	Anti-cancer	
110	Philip Michael Gance	05/2023-01/2024	Zika virus	Applying for Medical School
109	Sarah Misbah (BS, MCB)	01/2023-05/2023	Anti-cancer	Salus University, Master of Medical Science, Physician Assistant
108	Iman Moosvi (BS, Biology)	09/2022-01/2023	Anti-cancer	
107	AnneMarie Dominque (BS, Biology)	09/2022-05/2023	Anti-cancer	Applying for Medical School
106	Renz Joshua Aguilar (BS, Biology	Fall 2022	Anti-cancer	Applying for Medical School
105	Jiancalo Atienza (BS, MCB)	09/2022-05/2023	Anti-cancer	Medical technologist, Virtua
104	Andrew Stocklin (BS, Biochem)	09/2022-01/2023	Anti-cancer	
103	Clement Vu (BS, MCB)	09/2022-01/2024	Anti-cancer	
102	Claudine Marie Wrisley (BS, Biochem)	09/2022-01/2023	Anti-cancer	
101	Allison Zarro (BS, Bioinfo)	09/2022-01/2023	Anti-cancer	
100	Yaidaliz Medina (BS, Biochem)	09/2022-01/2023	Anti-cancer	
99	Gbemisola Olaoye (BS, Chem)	09/2022-01/2023	Anti-cancer	

98	Jared Briley (BS, Biochem)	09/2022-01/2023	Anti-cancer	
97	Savana Rodrigguez (BS, Biology)	09/2022-01/2023	Anti-cancer	Applying for Medical School
96	Sapna Modi (BS, Business)	09/2022-01/2023	Anti-cancer	
95	Andrew Robert (BS, Biochem)	09/2022-01/2023	Anti-cancer	
94	Jiancarlo Atienza (BS, Biology)	09/2022-05/2023	Anti-cancer	
93	Candice Bui-Linh (BS, Biology)	01/2022-05/2023	Anti-cancer	Applying for Medical School
92	Elizabeth Uzhca (BS, Biology)	01/2022-01/2023	Anti-cancer	
91	Akshay Gupta (BS, Biology)	01/2022-01/2023	COVID-19	Applying for Medical School
90	Mursalin Singh (BS, Biology)	01/2021-05/2023	COVID-19	Rowan University School of Osteopathic Medicine
89	Mark Christopher Alesiani (BS, Biology)	09/2020-05/2023	MMPL3	Applying for Medical School
88	Meeraj Amin (BS, Biology)	09/2020-05/2023	IL and COVID-19	Rowan University School of Osteopathic Medicine
60	Gilbert Fleischer (BS, Biology)	09/2019-05/2020	HBV, RdRp	Cooper Medical School of Rowan University
59	Stefi Lao (BS, Biochem)	09/2019-05/2020	CAR-T	Johnson & Johnson, CAR-T Manufacturing Operator
58	Jennifer Necsutu (BS, Biology)	01/2020-05/2020	GPCR	
57	John Vizzini	01/2018-05/2018	G-quadruplex	Doctor of Physical Therapy, Widner University
56	Jose Parra	01/2018-05/2018	GPCR	Associate of Pharmaceutical R&D, Ascendia Pharmaceuticals
55	Nazra Syed	01/2018-05/2018	GPCR	
54	Miranda Presiosi	01/2018-05/2018	GPCR	Organic Prep Technician, ALS
53	Joshua Freyer	01/2019-05/2019	SET 7	TMS Treater, Success TMS
52	Lucas Bennett	09/2018-05/2019	GPCR	Rowan Pharmaceutical Science (MS)
51	Dylan Brunt	09/2018-05/2019	GRCR	Rowan Pharmaceutical Science (MS)
50	Michael J. Pino	09/2018-05/2019	GPCR	Rowan Pharmaceutical Science (MS)

49	Nicolas Scorese	09/2014-05/2018	OTR receptor	MS, Bioinformatics, Rowan University. Data Analyst, PDS Life Sciences, Dean's Outstanding Senior Award 2018
48	Heral Patel	09/2017-05/2018	Way/TAAR1	Master's in Biomedical Sciences, Rutgers Robert Wood Johnson Medical School
47	Shaina Nogle	09/2017-05/2018	PPAR	Rowan Pharmaceutical Science (MS)
46	John Jacobson	08/2017-05/2018	GPCR receptor/Rhodopsin	
45	Alexandra Campbell	08/2017-05/2018	G-Quadruplex/HT1B	
44	Shane Scott	08/2017-05/2018	GPCR receptor/gP/Elastin	
43	Sarah Halim	08/2017-05/2018	Taxol/G-quadruplex	
42	Zachary Finkel	09/2017-05/2018	GPCR receptor/ILs	PhD, Biomedical Engineering, Rutgers University
41	Carina Olivas	08/2017-05/2018	TAAR1/	
40	Cecilia Floyd	09/2015-05/2018	Pain/Opioid receptor	Optometry Program, Salus University
39	Stephen Ahwin	09/2018-05/2019	GPCR	
38	John Alviar	09/2018-05/2019	GPCR	QC Chemist, Norquay Technogly
37	Ashleigh McConnell	09/2015-05/2018	Pain/Opioid receptor	
36	Holli-Joi Sullivan	01/2017-05/2018	Opioid receptor	Rowan Pharmaceutical Science (MS)
35	Victoria Persad	09/2017-05/2018	G-Quadruplex	
34	Adlin Antiquena	05/2017-05/2018	Opioid receptor	Analytical Chemist Adare Pharma Solutions
33	Nikkoli Lueder	06/2017-05/2018	GPCR receptor	Bioinformatics (MS), Rowan University
32	Michael Olivieri	05/2017-05/2018	Taxol analogs/taxol	Rowan Pharmaceutical Science (MS)
31	Jack Edward Perhach	01/2017-05/2018	M3 receptor	
30	Joseph Garner	06/2017-05/2018	G-quadruplex	
29	Farzana Siddiquei	01/2016-05/2017	G-quadruplex	Doctor of Dental Medicine, Temple University
28	Carolyn Readmond	05/2017-08/2017	PAR1/G-quadruplex	Department Best Biochemist Award

27	Amanda Tursi	01/2017-05/2017	HT1b receptor	Biomedical Informatics (PhD), University of Cincinnati, Bioinformatics (MS), University of Turku
26	Christina Radicella	09/2016-05/2017	OTR receptor	ASRC FEDERAL (software company)
25	David Montgomery	09/2016-05/2017	D2 receptor	PhD program in Univ. of Georgia
24	Thomas Fasano	09/2016-05/2017	G-quadruplex	Quality Control Lab Analyst, The Estée Lauder Companies Inc.
23	Lan Ge	01/2017-05/2017	GPCR receptor	Laboratory Technician, Bristol Myers Squibb
22	Jorge L. Moran-Nestor	01/2017-05/2017	GPCR receptor	GC Chemist, Atlantic Analytical Laboratory
21	Anna-Kay Tenn	01/2016-06/2016	GPCR receptor	
20	Alissa M. Yamabushi	01/2016-06/2016	GPCR receptor	Science Teacher, Penns Grove High School
19	Juan Sanchez Hernandez	01/2016-06/2016	GPCR receptor	
18	Matthew Crouch	07/2015-12/2016	D3 receptor	Calibrations Supervisor, Teligent Inc.
17	Christine Cancglin	09/2016-12/2016	Ionic Liquid	Johnson Matthey
16	Griffin Fountain	07/2015-12/2016	D4 receptor	Rowan Pharmaceutical Science (MS)
15	Matthew Gilmurray	09/2016-12/2016	D2 receptor	
14	Catherine Ann Deleon	07/2015-12/2016	TAAR1	Chemist, NAL Pharma
13	Jeffrey Maurer	02/2016-05/2016	Modeling/Simulation	Graduate Student, Bioinformatics, Boston University,
12	Alex Meremianin	02/2016-05/2016	Modeling/Simulation	Data Analyst at Oaks Integrated Care
11	John Davis Chea	02/2016-08/2017	Membrane receptor	PhD, Chemical Engineering, Rowan
10	Anna Caroline Gogola Muller	02/2016-05/2016	Allergy/H1	Specialist L.A. Centro De Ensino,
9	Gurmannat Kalra	02/2016-05/2016	Cancer/DNA quadruplex	PhD program in Univ. of Maryland
8	Iohana Bianca Pagnoncelli	02/2016-05/2016	Cancer/DNA quadruplex	Morphological Sciences (MS), Federal University of Rio de Janeiro

7	Abigail Marry Smith	02/2016-05/2017	Pain/Opioid receptor	Rowan Pharmaceutics Science (MS)
6	Fernanda Soares Rasquel De Oliveira	02/2016-05/2016	Diabetes/PPAR	
5	Paige Fisher	09/2015-05/2016	Pain/Opioid receptor	
4	Joshua Bartosz	*09/2015-12/2015*	Pain/Opioid receptor	Medical Technologist, Thomas Jefferson University Hospitals
3	Deirdra Mcneil	*09/2015-12/2015*	TAAR1	Rowan Bioinformatics Science (MS)
2	Anant Kumar	*05/2014-12/2015*	Membrane protein modeling	Science Writer at Getson & Schatz, P. C
1	Kevin O'Brien* (undergraduate)	*09/2013-09/2014*	Virtual drug screening	PhD program in Univ. of Pennsylvania
	High School Students			
	Bharat Elango	09/2022-present	Evolution of Flu Virus	2023 Coriell Institute Science Fair, 1st Place in Biochemistry
	Co-advising oversea graduate students			
3	Mingwei Wen (Ph.D student)	*2012-2014 /University of Chinese Academy of Sciences*	Modeling method development	Local Company
2	Zhanghang Chen (MS student)	*2013-2014/Shandong University*	Binding interactions between DNA and anti-cancer drugs	High School Teacher
1	Xiaolin Wang (Ph.D student)	*2013-2014/Shandong University*	Anti-microbial peptides	Faculty

SERVICE (UNIVERSITY COMMUNITY)

Departments

Fall 2022-present	Member, BBS Elections Committee
Fall 2021-present	Chair, Chem &Biochem Research Adjusted Load Committee
Fall 2020-present	Member, Chem & Biochem T & R Committee
Fall 2020-present	Member, Chem & Biochem Promotion Committee
Fall 2020-Spring 2021	Chair, MCB Promotion Committee
Fall 2019-Spring 2020	Member, MCB , Retention/Recruitment Committee
Fall 2019-Spring 2020	Member, MCB promotion Committee
Fall 2019-present	Member, Chem & Biochem T & R committee
Fall 2018-present	Member, M.S. Bioinformatics Grad Admissions Committee
Fall 2019-Spring 2020	Chair, MCB department T&R Committee Tenure package for Dr. Ben Carone T&R package for Dr. Yong Chen
Fall 2018-Spring 2019	Chair, MCB department T&R Committee Tenure package for Dr. Ileana Soto T &R package for Dr. Yong Chen T &R package for Dr. Marina Bogush
Fall 2017-Spring 2018	Chair, MCB department T&R Committee T&R 4th year packets for Dr. Ben Carone T&R package for Dr. Mary Alpaugh
Fall 2018-Spring 2019	Chair, Bioinformatics Faculty Search Committee (Dr. Yong Chen)
Fall 2018-Spring 2019	Bioinformatics Program Coordinator
Fall 2017	Chair, Bioinformatics Visiting Professor Search committee (Mr. John Malaron)
Fall 2017-Spring 2018	Chair, Biophysical Chemistry Faculty Search Committee (Dr. Erik Hoy)
Fall 2016	Presenter, Chemistry & Biochemistry New Student Orientation
Fall 2015- Fall 2016	Presenter, Translational Biomedical Sciences Open House
Fall 2015- Spring 2017	Presenter, Bioinformatics Open House
Spring 2015-Spring 2016	Presenter, Chemistry & Biochemistry Open House
Fall 2015-Spring 2016	Member, Health Data Analytics Faculty Search Committee
Fall 2014	Member, Task Force: ASBMB accreditation of biochemistry program
Fall 2014	Member, Task Force for Rutgers Rowan Center Biomedical Research
Fall 2013-Spring 2014	Member, Pharmacology Faculty Search Committee
Fall 2013-Spring 2014	Member, Neuroscience Faculty Search Committee
Fall 2013-present	Administrator, license servers for Schrodinger, Mestrelab and Spartan
Fall 2013-present	Renewal for ChemOffice, Schrodinger and Spartan
Fall 2013-present	Administrator, Software installation, 56 department laptop computers

College

Fall 2021-Present	Member	Neuroscience BS Program Development Committee
Fall 2021-Spring 2022	Member	CSM T&R Committee
Fall 2021-Spring 2022	Member	CSM Research Adjusted Load Committee
Spring 2017	Presenter	Virtual reality VR presentation on CADD and Faculty Roundtable Dr. Ulo Palm (Allergan) Dean's Distinguished Speakers Series
Spring 2017	Receptionist	Nanyang Normal University Delegation
Spring 2017	Presenter	Rowan University Science Day
Spring 2016	Presenter	Rowan University Science Day
Spring 2015	Presenter	Rowan University Science Day
Spring 2014	Receptionist	Korean graduate student delegation (5 Korean students)
Fall 2013-Spring 2014	Member	CSM Computational Center Grant Team

University

Fall 2022-Spring 2023	Member	Senate Research Committee
Spring 2019	Reviewer	Rowan SEED award
Fall 2016-Spring 2017	Member	Senate Bookstore Committee
Spring 2020-present	Member	Core Leadership Team for NSF Campus Cyberinfrastructure Star program
Spring 2016-present	Member	HPC@Rowan committee

High-Performance Computer (HPC) @ Rowan

As co-PI and a member of the, I have played a critical role in establishing this HPC facility using my unique HPC expertise (only investigator had built and managed a HPC cluster.):

- Critical suggestion on the hardware configuration/architecture of this HPC
- Critical suggestion on the software configuration and queue policy
- Critical suggestion on User Policies
- Important suggestion on User Education and Outreach
- Testing and benchmarking this HPC

This HPC provides a critical infrastructure in actively transforming Rowan to a true research university. This HPC will not only enhance research in existing areas of excellence, such as machine learning, biomedical research and geotechnical engineering, but will also expand support for the emerging areas of bioinformatics, dynamic systems optimization and environmental sustainability research. This HPC is a university-wide shared resource that will be a focal point for strengthening and extending existing research and collaborations and will serve as a platform for developing new research and educational initiatives.

Thesis/Dissertation Committees

Fall 2024	Member	PhD Pharmaceutical Sciences	Indu Mithra Madhuranthakam
Spring 2024	Member	MS Pharmaceutical Sciences	Julia Q, Gabriel
Spring 2024	Chair	MS Pharmaceutical Sciences	Justin D. Carbone
Spring 2024	Chair	MS Pharmaceutical Sciences	Mariya Hryb
Fall 2023	Member	MS Pharmaceutical Sciences	Austin Clark
Fall 2023	Member	MS Bioinformatics	Madison A. Dautle
Spring 2022	Chair	MS Pharmaceutical Sciences	Nicholas J. Paradis
Spring 2022	Chair	MS Pharmaceutical Sciences	Emily Dean
Spring 2022	Member	MS Pharmaceutical Sciences	Ashka Patel
Spring 2021	Member	PhD Biochemical Engineering	Robert Mosley
Spring 2021	Member	MS Bioinformatics	Sadegh Majdi
Spring 2021	Chair	MS Pharmaceutical Sciences	Griffin Fountain
Spring 2020	Member	MS Pharmaceutical Sciences	Alexandria Senetra
Spring 2020	Chair	MS Bioinformatics	Brian Chen
Spring 2020	Member	MS Pharmaceutical Sciences	Mohammad A. Rahman
Spring 2020	Chair	MS Pharmaceutical Sciences	Holli-Joi Sullivan
Spring 2019	Chair	MS Bioinformatics	Nicolas Scorese
Fall 2018	Member	MS Pharmaceutical Sciences	Hannah Hoag
Fall 2018	Member	MS Pharmaceutical Sciences	Xiaotian Chen
Spring 2018	Member	MS Pharmaceutical Sciences	Ariful Islam
Spring 2017	Chair	MS Pharmaceutical Sciences	Babitha Machireddy
Spring 2017	Member	MS Pharmaceutical Sciences	Keyur Pandya
Spring 2017	Member	MS Pharmaceutical Sciences	Bhawan Patel
Spring 2016	Chair	MS Pharmaceutical Sciences	Safaa Sader
Spring 2016	Chair	MS Bioinformatics	Kelly Mulholland
Spring 2016	Member	MS Bioinformatics	Andrea Burke

SERVICE (WIDER AND PROFESSIONAL COMMUNITY)

Professional Memberships

- American Chemical Society (ACS) (2009-present)
  - Presented 18 talks at ACS national meetings (2017 Fall/3, 2018 Spring/1, 2019 Spring/1, 2020 Spring, 2021 Spring/1, 2021 Fall/5, 2022 Spring/4 and 2022 Fall/3)
  - Presented one talk at the 2019 Middle Atlantic Regional Meeting

- American Biophysical Society (2009-present)
  - Presented one talk at 61st Annual Meeting (2017)

International Scholar and Research Exchange

- Served as an Associate Member to Beijing Computational Science Research Center, 2018-2022
  - Served to review to research proposals as external expert
  - Served to evaluate annual performance of postdocs at CSRC as external expert
  - Collaboration with Prof. Haiguang Liu

- Distinguished contribution to the World Class Professor program by Indonesia Ministry of Education and Culture, Republic of Indonesia, by collaborating with Dr. Muhammad Arba in research and by offering a series of 10 research lectures for 20 students from Faculty of Pharmacy, Universitas Halu Oleo. Fall 2021

- Hosted three visiting professors from China (Prof. Kai Tan, Prof. Xiaoyan Wang, Prof Liao Siyan), leading 7 joint publications, 2015-2021

- I visited several universities and institutions in China to give research talks as well as to promote our MS Pharmaceutical Sciences program and MS Bioinformatics program. Some of the institutes that I visited include Xiamen University (2019), Fudan University (2018), Zhejiang University (2018), Yunnan University (2018), Daping Hospital, Army Medical University (2018), Sichuan University (2018), Guangzhou Medical University (2018), Sun Yat-Sen University (2018), School of Pharmaceutical Sciences, Xiamen University (2018), Nanjing University (2018), Beijing University (2018), Beijing Normal University (2018), Beijing University of Posts and Telecomunications (2018)

Organized research workshops

- Workshop “Computer Aided Drug Design (CADD) techniques”, WCP program of Indonesia Ministry of Education and Culture, Republic of Indonesia, Faculty of Pharmacy, Universitas Halu Oleo. Fall 2021
- Workshop “Computer Aided Drug Design (CADD) methods”, School of Pharmaceutical Sciences, Xiamen University, China, August 19-23, 2019
- Workshop “Computer Aided Drug Design (CADD) techniques”, Beijing Computational Research Sciences Center (CRSC), Beijing, China August 6-12, 2019
- Workshop “Theoretical and computation biology: from molecules to systems”, Songshan Lake in Dongguan, China, August 1-4, 2019
- Workshop “Computer Aided Drug Design (CADD) method”, Beijing Computational Research Sciences Center (CRSC), China, July 10-14, 2018

Reviewer for 40+ Scientific Journals

- Nature Chemistry
- Journal of American Chemical Society,
- Journal of Molecular Biology
- Biophysics Journal
- Journal of Physical Chemistry

- Biopolymer
- Biophysical Chemistry
- Physical Chemistry Chemical Physics
- PLoS ONE,
- Proteins: Structure, Function and Bioinformatics,
- Protein Science,
- Scientific Reports
- Current Computer-Aided Drug Design,
- Genomics, Proteomics & Bioinformatics
- Cellulose
- Science China Chemistry
- Journal of Solution Chemistry
- Journal of Molecular Graphics and Modeling
- Journal of Theoretical and Computational Chemistry
- Letter in Drug Design and Chemistry
- Anticancer Agents in Medicinal Chemistry
- Heliyon
- Journal of Molecular Graphics and Modelling
- Pharmaceutics
- International Journal of Physics Research
- Computational and Structural Biotechnology Journal
- Food Science and Human Wellness
- Viruses
- Chemistry - A European Journal
- Journal of Addiction Therapy and Research
- Environmental Science and Pollution Research
- Chemical Data Collections
- Journal of Infection and Public Health
- Annals of Gerontology and Geriatric Research
- Biomolecules
- Nucleosides, Nucleotides & Nucleic Acids
- ACS Chemical Neuroscience
- Arabian Journal of Chemistry
- Bioorganic & Medicinal Chemistry
- Biochimie

Some recent journal articles that I reviewed are as follows:

1. **Biochimie**, Prevention of Insulin aggregation by biocompatible choline-amino acid based ionic liquids: Biophysical insights Biochimie, 2022
2. **Arabian Journal of Chemistry**, Interactions and effects of natural isoquinoline alkaloid palmatine with DNA: Inference and validation based on computational chemistry, bioinformatics and biological experiments, 2022
3. **Molecules**, Aldose reductase inhibitory potentials of xanthones isolated from African medicinal plants: A Computational Approach, 2022
4. **Bioorganic & Medicinal Chemistry**, Design, Synthesis and Evaluation of Inhibitors of the SARS-CoV2 nsp3 Macrodomain, 2022
5. **Arabian Journal of Chemistry**, LC-MS Profiled Chemical Constituents, Molecular Modeling, and In vitro Bioactivity Evaluations of Suaeda vermiculata Extracts as Anti-Hepatocellular Carcinoma Preparation: Assessment of the Constituents' Role, and Receptor Docking Feasibility Based Activity Projections, Arabian Journal of Chemistry 2022
6. **ACS Chemical Neuroscience**, Critical extracellular Ca2+ dependence of the binding between PTH1R and a G protein peptide revealed by MD simulations, 2022
7. **Nucleosides, Nucleotides & Nucleic Acids**, Interaction of the platinum complex of tyrosine-β-cyclodextrin with G-quadruplex DNA, 2022

8. **Biomolecules**, Synthesis and Effect of Conformationally Locked Carbocyclic Guanosine Nucleotides on Dynamin Special Issue: Pharmacology of Purinergic Receptors, 2022
9. **Annals of Gerontology and Geriatric Research**, Association of Potentially Inappropriate Medication and potential drug interactions with Toxicity and Adherence to Anti-Neoplastic Treatment. 2022
10. **Journal of Infection and Public Health**, Receptor Binding Domain of SARS-CoV-2 from Wuhan Strain to Omicron B.1.1.529 attributes increased affinity to variable structures of Human ACE2, 2022
11. **Computational and Structural Biotechnology Journal**, Recognition of the Ligand-Induced Residue Pattern of β2-Adrenergic Receptors Using 3D-ResNets Trained by the Time Series of Protein Distance Maps, 2022
12. **Journal of Molecular Graphics and Modelling**, Exploring the multiple conformational states of RNA Genome through interhelical dynamics and network analysis, 2022
13. **Chemical Data Collections**, Molecular Docking and Dynamics Simulation of Several Flavonoids Predict Cyanidin as an Effective Drug Candidate Against SARS-CoV-2 Spike protein, 2022
14. **Environmental Science and Pollution Research**, Efficacy of Selected Nigerian Tropical Plants in The Treatment of COVID-19: In silico and in vitro investigations,2022
15. **Journal of Addiction Therapy and Research**, A qualitative study on the leadership traits of people with substance use disorder, 2022
16. **Chemistry - A European Journal**, Deciphering the Interactions Between Small Molecules and G-Quadruplex DNA, 2022
17. **The Journal of Physical Chemistry**, Effects of Familial Alzheimer's Disease Mutations on the Folding Free Energy and Dipole-Dipole Interactions of the Amyloid β-Peptide, 2022
18. **Viruses**, Structural Analysis and Molecular Dynamics simulation studies of HIV-1 Antisense Protein (ASP) predicts its potential role in HIV replication and pathogenesis, 2022
19. **Food Science and Human Wellness**, Mulberrofuran G, a mulberry component, prevents SARS-CoV-2 infection by blocking the interaction between SARS-CoV-2 spike protein S1 receptor-binding domain and human angiotensin-converting enzyme 2 receptor, 2022
20. **Computational and Structural Biotechnology Journal**, Identifying binding sites to target the Receptor-Binding Domain of SARS-CoV-2 Spike protein, 2022
21. **International Journal of Physics Research**, Oscillation of Neutrino in a Vacuum with Mixing Flavor
22. **The Journal of Physical Chemistry**, Modelling Peptide Nucleic Acid (PNA) Binding Enthalpies using MM-GBSA, 2022
23. **Pharmaceutics**, Cheminformatic identification of phenolics as modulators of penicillin-binding protein 2a of Staphylococcus aureus: a structure-activity relationship-based study Special Issue: In Silico Pharmacology for Evidence-Based and Precision Medicine, 2022
24. **Journal of Molecular Graphics and Modelling**, Biased agonists differentially modulate the receptor conformation ensembles in Angiotensin II Type 1 Receptor, 2022
25. **Heliyon**, Deep learning-based Drug discovery of Mac domain of SARS-CoV-2 (WT) Spike inhibitors: using experimental ACE2 Inhibition TR-FRET Assay Screening and Molecular Dynamic Simulations, 2022
26. **Physical Chemistry Chemical Physics**, A multiple-step in silico screening protocol to identify allosteric inhibitors of Spike-hACE2 binding, 2022
27. **Physical Chemistry Chemical Physics**, Structural Insights Into Nirmatrelvir (PF-07321332)–3Clike SARS-CoV-2 Protease Complexation: A Ligand Gaussian Accelerated Molecular Dynamics Study
28. **Frontiers in Pharmacology**, Critical sites influencing ligand bias at μ-opioid receptor, 2022
29. **The Journal of Physical Chemistry**, Mechanistic insights into the co-aggregation of Aβ and hIAPP: an all-atom molecular dynamic study, 2021
30. **Chemical Biology &Drug Design**, Structure-based Derivation and Optimization of YAP-like Coactivator-derived Peptides to Selectively Target TEAD Family Transcription Factors by Hydrocarbon Stapling and Cyclization, 2022
31. **The Journal of Physical Chemistry**, *Impact of Au144 Metal Clusters on the Structural and Inhibitory Mechanism of Aβ42 Peptide: A Theoretical Approach,* 2020
32. ***Journal of Biomolecular Structure & Dynamics**, Dopamine Molecular Channels,* 2020
33. ***Physical Chemistry Chemical Physics**, Unexpected adsorption feature of polynucleotide ssDNA molecules on graphene oxide,* 2020

34. **The Journal of Physical Chemistry***, Nucleation-Dependent Aggregation of Human Prion Peptides: Insights from Atomistic Molecular Dynamics Study*, 2020
35. ***Physical Chemistry Chemical Physics****, Importance of crystalline water network in docking-based virtual screening: a case study of BRD4, 2019*
36. **The Journal of Physical Chemistry***, Modeling of Fibrillation Induced Selective Cytotoxicity of Cross-α Amyloid – Phenol Soluble Modulin α3*, 2019
37. **Physical Chemistry Chemical Physics**, *Multiple folding pathways of the villin headpiece subdomain HP35*, 2019
38. **Molecules**, Ligand Selectivity in the Recognition of 1 Protoberberine Alkaloids by Hybrid-2 Human 2 Telomeric G-Quadruplex: Binding Free Energy 3 Calculation and NMR Experiment, 2019
39. **The Journal of Physical Chemistry***, "Caffeine Destabilizes Preformed Aβ Protofilament: Insights from All Atom Molecular Dynamics Simulations",* 2019
40. **The Journal of Physical Chemistry***, "All-Atom Structure Ensembles of Islet Amyloid Polypeptides Determined by Enhanced Sampling and Experiment Data Restraints",* 2018
41. **Journal of Molecular Graphics and Modelling**, "Pharmacoinformatics Analysis of Merbarone Binding Site in Human Topoisomerase IIα", 2018

Reviewer for external grant proposals

CSSI and MRI program of NSF in 2019 and in 2016
Starting Grant proposals for European Research Council (ERC) in 2015

Member of editorial boards

Current Computer-Aided Drug Design, Frontiers in Catalysis, Journal of Applied Solution Chemistry and Modeling, Biomolecules Molecular Structure and Dynamics section of Biomolecules, Journal of Medicinal Chemistry and Drug Design

Executive Summary

Chun Wu

Associate Professor, Chemistry and Biochemistry, Biological Biomedical Sciences

Teaching Effectiveness

- In this promotion, I have taught 11 courses (Biochemistry, Bioinformatics-Biochemical applications, Biophysical Chemistry, Survey of Molecular Modeling Methods, Seminar, Advanced Biochemistry, Advanced Bioinfo-Biochem applications, Advanced Biophysical Chemistry, Advanced Surv of Mol Modeling Methods, Advanced Biochemistry Lab, Translational Biomedical Research I-IV). The student evaluation was collected for Biochemistry from Summer 2021 (**4.61/5.0**) and Summer 2022 (**4.58/5.0**) and Advanced Bioinfo-Biochem applications from Fall 2021 (**4.31/5.0**). This cycle's average score is **4.5/5.0** (3 courses), which is **0.24** higher than the average score (**4.26/5.0**) from prior cycles (16 courses).
- I developed a series of on-line dry labs to replace the original wet labs for Biochemistry and Biophysical Chemistry, enabling smooth transition to Hybrid classes due to COVID-19 for all sections of these courses.
- I contributed to the development of an upper level course (Applications in Experimental and Computational Chemistry) and the upgrade of Advanced Biochemistry Lab and the Neuroscience BS Program/Computational Track.
- I supervised 30 MS graduate students (17 in this promotion) in research leading to 36 publications and 69 posters (28 publications and 53 posters in this promotion) with the graduate students listed as co-authors. 14 out of the 30 graduate students are from underrepresented group in science and engineering. One poster presentation received student poster award at 2021 MidAtlantic Bioinformatics Conference.
- I supervised 99 undergraduate students (63 in this promotion) in research leading to 30 publications and 83 posters (23 publications and 35 posters in this promotion) with the undergraduate students listed as co-authors. 59 out of the 99 undergraduate students are from underrepresented group in science and engineering. Two women students won the department research awards.
- The accomplishments of my alumni in the past ten years include: one student finished postdoc study, 8 MS students joined PhD programs and 13 MS students joined various companies, 23 BS students joined graduate schools including medical schools, dental schools, pharmacy schools, optometry program, physical therapy etc. and 17 joined various companies.
- Wrote 75 recommendation letters for students

Scholarly and Creative Activity

- Established a Computer-Aided Drug Design (CADD) lab with 14 workstations, 5 GPU workstations, a high performance cluster (HPC) cluster with 288 CPUs.
- Published 41 peer-reviewed papers and 1 peer-reviewed book chapter (as a leading/corresponding author on 29 of 40 publications) in this promotion. 45% of my entire publications (~92 since 2000) were completed after my tenure. 36 out of the 41 journal articles were published in Q1 journals (Top 25% journals in their specific research category), and 36 were published in journals with a 2022 impact factor higher than 3. According to Google Scholar, my publications have been cited more than 8478 times in total, with h-index=33, i10-index= 58.
- Wrote 20 grant proposals, with 13 awarded, 4 pending (2 as PI and 2 as Co-PI/Senior investigator) for ~$1M and 3 unfunded in this promotion.
- Awarded 1.1 million dollars (0.67 million as PI and 0.43 million as Co-PI) in research funding from external sources from the 13 awards in this promotion. Among $1,105,815, $300,000 is from National Science Foundation, $100,000 is from industry, and $100,000 is foreign Institution, $70,000 is from New Jersey Health Foundation, Supercomputer Time (6x200,000 SUs) with equivalent value based on Amazon EC pricing $262,440 from National Science Foundation, the fastest supercomputer anton 2 time for molecular dynamics simulation (100,000+150,000 MD Simulation Units) with equivalent dollar value ($273,375) from National Research Council at the National Academies of Science. Anton 2 is ~180 times faster than any general-purpose supercomputer. I was Awarded a total of 2.0 million dollars (1.1 million as PI and 0.9 million as Co-PI) in research funding from external sources since my joining Rowan in 2013.

- Gave 16 oral talks at American Chemical Society (ACS) national meetings (14), regional meetings (2) in this promotion.
- Gave 19 invited talks at academic institutions (19) in this promotion.
- Presented 50 posters at ACS national (4), regional (3) and local meetings (43) in this promotion.
- Mentored 2 postdocs and 3 visiting scholars (2 posdocs and 1 visiting scholar in this promotion) in research leading to 18 publications (16 in this promotion) with the postdocs and the visiting scholars listed as co-authors
- Established research collaboration with 13 research groups including 9 Rowan research groups (Drs. Greg Caputo, Timothy Vaden, Subash Jonnalagadda, Xiaoyang Mou, Claude Krummenacher, Thomas Keck, Lark Perez, Gustavo Moura-Letts, Xiao Hu, Manoj Pandey, Dimitri Pestov) and 6 groups from Beijing CSRC, Xiamen University, the ohio state university, Shandong university, Ocean University of China, Graduate University of Chinese Academy of Sciences

Contribution to University Community

- Provided peer course assessments for faculty in both Chem & Biochem and MCB department
- Member, BBS Department Elections Committee, 2022
- Chair, Chem & Biochem Department Adjusted Load Committee (2021-2022)
- Member, Chem & Biochem T & R Committee, Promotion Committee (2019-2022)
- Chair, MCB Promotion Committee, 2020
- Member, MCB , Retention/Recruitment Committee, promotion Committee 2019
- Member, M.S. Bioinformatics Grad Admissions Committee 2018-2022
- Chair, MCB department T&R Committee 2017-2019
- Chair, Bioinfo Faculty/Bioinfo Visiting Professor/ Biophy Chem Faculty Search Committee 2017-2018
- Bioinformatics Program Coordinator, 2018
- Administrator for departmental chemistry softwares (2013-2022)
- Member, CSM T&R Committee, 2021
- Member, CSM Research Adjusted Load Committee, 2021
- Member, Neuroscience BS Program Development Committee, 2022
- Reviewer, Rowan SEED award, 2019
- Member, Senate Bookstore Committee, 2017
- Member, Core Leadership Team for NSF Campus Cyberinfrastructure Star program
- Member, High-Performance Computer (HPC) @ Rowan committee
- Member, 10 MS Thesis Defense Committees in CSM
- Member, 1 PhD Thesis Defense Committees in Engineering College

Contribution to Wider and Professional Community

- Member, in American Chemical Society (ACS) and Biophysical Society since 2009
- Presented 18 talks at ACS national meetings (2017 Fall/3, 2018 Spring/1, 2019 Spring/1, 2020 Spring, 2021 Spring/1, 2021 Fall/5, 2022 Spring/4 and 2022 Fall/3)
- Presented one talk at the 2019 ACS Middle Atlantic Regional Meeting
- Presented one talk at 61st Biophysical Society Annual Meeting (2017)
- Served as Associate Member for Beijing Computational Science Research Center (CSRC) 2018-2022
- Selected by the World Class Professor program by Indonesia Ministry of Education and Culture, Republic of Indonesia, 2021
- Hosted three visiting professors from China (Prof Liao Siyan, Prof. Kai Tan and Prof. Xiaoyan Wang), 2015-2021
- visited several universities and institutions in China to give research talks as well as to promote our MS Pharmaceutical Sciences program. Some of the institutes that I visited include Xiamen University (2019), Fudan University (2018), Zhejiang University (2018), Yunnan University (2018), Daping Hospital, Army Medical University (2018), Sichuan University (2018), Guangzhou Medical University (2018), Sun Yat-Sen University (2018), School of Pharmaceutical Sciences, Xiamen University (2018),

Nanjing University (2018), Beijing University (2018), Beijing Normal University (2018), Beijing University of Posts and Telecomunications (2018)

- Organized several workshops on Computer Aided Drug Design
- Served as reviewer for 40+ journals and performed peer reviews for 41+ manuscripts