

Department of Chemistry
Purdue Institute for Drug Discovery
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EDUCATION

- 2003-2010 **Stanford University, Stanford, CA**
M.S. in Scientific Computing/Computational Mathematics, May 2005
Ph.D. in Computational Mathematics, January 2010
- 2002-2003 **University of California at Irvine, Irvine, CA**
M.S. in Mechanical and Aerospace Engineering, May 2003
- 1998-2002 **Indian Institute of Technology – Delhi, New Delhi, India**
B. Tech. in Mechanical Engineering, May 2002

ACADEMIC EXPERIENCE

- 2020-present **Director, Merck-Purdue Center for Measurement Science**
Merck sponsored center funding research projects across Purdue University
Total investment by Merck at Purdue till date = **\$1,336,185**
<https://www.science.purdue.edu/merck/leadership.html>
- 2022-present **Associate Professor (tenured)**
2016-2022 **Assistant Professor (tenure-track)**
Purdue University, Department of Chemistry, West Lafayette, IN
- 2021-present Purdue University, Department of Computer Science (*by Courtesy*), West Lafayette, IN
Full Member: Purdue Center for Cancer Research
Affiliations: Purdue Institutes for Drug Discovery Integrative Neuroscience, Immunology, Integrative Data Science Initiative, Computational Life Science, Bindley Bioscience Center, PULSe
Research Area: **Chemical and Cellular Immunology**
- 2013-2016 **JDRF Postdoctoral Fellow**
University of California – San Francisco, Diabetes Center, San Francisco, CA
Mentor: Professor Jeffrey A. Bluestone
Research Area: Cellular Immunology
- 2010-2012 **Postdoctoral Scholar**
Stanford University School of Medicine, Department of Structural Biology, Stanford, CA
Mentor: Professor Michael Levitt (*2013 Nobel Laureate in Chemistry*)
Research Area: Drug Discovery
- 2005-2010 **Graduate Research Assistant**
Stanford School of Engineering, Computational Math/Biology/Chemistry, Stanford, CA

Mentor: Professor Michael Levitt (2013 Nobel Laureate in Chemistry)
Research Area: Computational Chemistry and Biology
Dissertation: Computational Modeling of Solvent in Structural Biology

2003-2005 **Graduate Research Assistant and Programmer**
Stanford School of Earth, Energy and Environmental Sciences, Stanford, CA
Mentor: Professor David D. Pollard

2002-2003 **Graduate Research Fellow**
University of California at Irvine, Mechanical and Aerospace Engineering
Mentor: Professor Marc J. Madou

AWARDS AND HONORS

2022 NIH NCATS ASPIRE Reduction to Practice Award (Stage 2 Milestone 2)
2021 **Two** NIH NCATS ASPIRE Reduction to Practice Awards (Stage 1, Stage 2 Milestone 1)
2020 Undergraduate Advising Award, Purdue College of Science, Purdue University
2019 NIH NCATS ASPIRE Challenge #1 Award (NIH HEAL Initiative)
2019 NIH NCATS ASPIRE Challenge #3 Award (NIH HEAL Initiative)
2018 Teaching for Tomorrow Fellowship Award
2018 Digital Education Award for Online Course Development
2018 Honorarium and Invited Seminar, *Merck & Co.*
2017 Institute Seminar and Honorarium at *National Center for Biological Sciences*, India
2017 Ralph W. and Grace M. Showalter Research Trust Award
2017 Jim and Diann Robbers Research Award for New Investigators
2016 Instructional Innovation Award, Purdue University
2016 Grand Rounds Seminar and Honorarium at *Eli Lilly & Company*, IN, USA
2013-2016 Juvenile Diabetes Research Foundation (JDRF) Award

CONSULTING AND SCHOLARLY ASSOCIATIONS

2019-present Consultant, Deciduous Therapeutics Inc.
2019-present Member, American Society for Mass Spectrometry (ASMS)
2017-present Member, Society for Neuroscience (SfN)
2017-present Member, American Association of Immunologists (AAI)
2016-present Nominated member, American Association for Cancer Research (AACR)
2016-present Member, American Chemical Society (ACS)
2016-present Member, Biophysical Society
2016-present Nominated member, Sigma Xi
2014-present Member, International Society for Computational Biology (ISCB)
2016-2018 Member, American Association for the Advancement of Science (AAAS)
2016-2017 Member, The New York Academy of Sciences
2010-2015 Structural Genomics Section of the Structural Biology Faculty of 1000

FUNDING

*Total Awards Amount: \$ 10,941,078 (Start-up **not** included; Awards < \$5,000 **not** shown in list below)*
from Department of Defense, National Institutes of Health, National Science Foundation, Office of Naval

Research, The Geneva Foundation, National Institute of Food and Agriculture, Merck & Co., Agilent Technologies, Indiana Bioscience Research Institute, Indiana CTSI, Showalter Trust, Integrative Data Science Institute, Purdue Center for Cancer Research, Purdue Institute for Drug Discovery, Purdue Provost Office.

External Funding

National Institutes of Health 07/15/2022 – 05/31/2024

1U18TR004146-01

National Center for Advancing Translational Science (NCATS)

Chemical instruments-aware distributed blockchain based open AI platform to accelerate drug discovery

Role: PD/PI

Total requested: \$1,073,736

Department of Defense 08/01/2020 - 07/31/2023

W81XWH-20-1-0665

Congressionally Directed Medical Research Programs - Peer Reviewed Alzheimer's Research Program

Elucidating Microglial Immune Regulation Targets to Remove Protein Aggregates in TBI

PI/PD

Total award: \$1,300,000

National Institutes of Health 09/01/2021 - 08/31/2024

1R01MH128866-01

Development of a high throughput system for molecular imaging of different cell types in mouse brain tissues

Multi-PI (PD: Julia Laskin, Purdue University)

Role: PI

Total award: \$1,551,433

National Science Foundation 08/01/2020 - 07/31/2023

NSF-2004102

D3SC: Signaling Axes Modulated by Cyclic Dinucleotides

PI/PD

Total award: \$444,000

Department of Defense 09/15/2021 – 09/14/2023

W81XWH-21-1-0891

Congressionally Directed Medical Research Program, Duchenne Muscular Dystrophy Research Program

Ligand-assisted delivery of immunoregulatory agents to dystrophic muscle for repeat dosing of AAV-dystrophin gene therapy

Multi-PI (PD: S. Armando Villalta, UC Irvine Medicine, *Subaward*)

Role: co-PI/PD, \$173,707

Total award: \$350,000

National Institutes of Health 06/01/2021 - (*unrestricted funds*)

National Center for Advancing Translational Science ASPIRE Reduction-to-Practice Challenge

*Iterative learning and automated modular platform for optimum non-addictive analgesic discovery**

Role: PI/PD

Total prize: \$1,220,000 (Stage 1 = \$120,000; Stage 2, Milestone 1 = \$150,000; Stage 2, Milestone 2 = \$200,000; Stage 3 = \$750,000)

* Funded for Stage 1 – Prize = \$120,000

* Funded for Stage 2, Milestone 1 – Prize = \$150,000

* Funded for Stage 2, Milestone 2 – Prize = \$200,000

<https://ncats.nih.gov/aspire/funding/2020ChallengeWinners>

National Institutes of Health

06/01/2021 - (unrestricted funds)

National Center for Advancing Translational Science ASPIRE Reduction-to-Practice Challenge
*Accelerating Molecular Innovation in Pain through an AI-driven Human-guided and Automated Open Drug Discovery Platform**

Role: PI

PD: Indiana Bioscience Research Institute

Total prize: \$1,220,000 (Stage 1 = \$120,000; Stage 2, Milestone 1 = \$150,000; Stage 2, Milestone 2 = \$200,000; Stage 3 = \$750,000)

* Funded for Stage 1 – Prize = \$120,000

* Funded for Stage 2, Milestone 1 – Prize = \$150,000

<https://ncats.nih.gov/aspire/funding/2020ChallengeWinners>

National Institute of Food and Agriculture (NIFA)

09/01/2020 - 08/31/2023

United States Department of Agriculture

A Pathogen-safe Sorter for the Center for Food Safety Engineering at Purdue University

Co-PI (PD: Paul J. Robinson, Purdue U.)

Total award: \$500,000

National Science Foundation

04/01/2020 - 03/31/2023

REU Site: Analyze This: Analytical Chemistry Applied to Interdisciplinary Research

Co-PI (PI: Greg Michalski, Purdue U.)

Total award: \$300,000

National Institutes of Health

01/01/2020 - (unrestricted funds)

National Center for Advancing Translational Science (NCATS) ASPIRE Design Challenge
Integrated Chemistry Database for translational Innovation in Pain, Opioid Abuse Disorder and Overdose

PI/PD, \$90,000

Total award: \$100,000

National Institutes of Health

01/01/2020 - (unrestricted funds)

National Center for Advancing Translational Science (NCATS) ASPIRE Design Challenge
Optimum Analgesic Discovery by Multiscale Interatomic Profiling

PI/PD, \$50,000

Total award: \$100,000

National Institutes of Health

09/04/2018 - 09/03/2023

5T32DK101001-08

National Institute of Diabetes and Digestive and Kidney Diseases (NIDDK)
Interdisciplinary Bioengineering Training in Diabetes Research (T32)

Co-I (PD: Sherry Voytik-Harbin, Purdue U.)

Total award: \$1,359,000

<p>Office of Naval Research <i>Robust Fuel Composition Analysis for Resilient Logistics</i> Co-PI (PI/PD: Gozdem Kilaz, Purdue U.) Total award: \$249,995</p>	<p>04/01/2020 - 03/31/2022</p>
<p>Department of Defense AFOSR – Air Force Office of Scientific Research, Control # 21RT0548 <i>Nano-Needle Bioelectronics: soft intracellular electrodes for mapping the sub-cellular neural code</i> Role: co-PI (PD: Jayant Krishna, Biomedical Engineering, Purdue University) Total requested: \$321,356</p>	<p>02/01/2022 - 01/31/2023</p>
<p>Merck & Company Inc. <i>Assay Development and Optimization to Differentiate Immune Response Induced by Vaccination and Natural Viral Infection</i> PI/PD Total award: \$55,000</p>	<p>05/01/2021 - 04/30/2022</p>
<p>Indiana Clinical & Translational Science Institute <i>Design and Synthesis of Next Generation 12-Lipoxygenase Inhibitors for Prevention and Treatment of Diabetes</i> PI/PD (Purdue), \$33,552 Total award: \$75,000</p>	<p>06/01/2019 - 04/30/2022</p>
<p>Department of Defense The Geneva Foundation, S-1424-02 <i>Modeling Molecular Mechanisms of Pirfenidone Interaction with Kinases</i> PI/PD Total award: \$209,000</p>	<p>09/30/2020 – 09/29/2021</p>
<p>National Science Foundation I/UCRC Center for Bioanalytic Metrology <i>Fully Autonomous HPLC/MSⁿ Interpretable Machine Learning Platform</i> PI/PD Total award: \$100,000</p>	<p>01/01/2021 - 12/31/2021</p>
<p>Merck & Company Inc. <i>Machine Learning Framework for Bioanalytical Method Development and Automation</i> PI/PD Total award: \$75,000</p>	<p>08/01/2020 - 07/31/2021</p>
<p>National Science Foundation I/UCRC Center for Bioanalytic Metrology <i>Molecular Identification using Machine Learning and MRM Profiling</i> PI/PD Total award: \$100,000</p>	<p>01/01/2020 - 06/30/2021</p>
<p>Indiana Clinical & Translational Science Institute <i>Identifying Molecular Targets Modulating Microglial Phagocytosis of Amyloid-beta</i></p>	<p>01/01/2020 - 06/31/2021</p>

PI/PD
Total award: \$40,756

Merck & Company Inc. 08/23/2019 - 12/31/2020
Machine Learning Methods to Elucidate Peptide Aggregation
PI/PD
Total award: \$50,000

National Science Foundation 06/01/2020 - 11/30/2020
Accelerating Understanding of COVID-19 Biology and Treatment via Scaled Medical Record and Biosimulation Analytics
PI (Purdue) (SBIR Phase I; PD: Guha Jayachandran, Onu Technologies Inc.)
Total award: \$256,000

Agilent Technologies 07/01/2020 – (unrestricted access)
Agilent 6495C Triple Quadrupole LC/MS Instrument
Agilent HPLC System – 1290 Infinity II LC System
PI/PD, Instrument Gifts for exclusive use in my lab (\$500,000)

National Science Foundation 05/01/2016 - 08/31/2019
REU Site: Analyze This: Analytical Chemistry Applied to Interdisciplinary Research
Co-PI (PI: Greg Michalski, Purdue U.)
Total award: \$300,000 (Renewed for 04/01/2020 - 03/31/2023 as listed above)

Indiana Bioscience Research Institute 09/01/2018 - 09/11/2019
Repurposed or Novel Inhibitors that Drive Beta Cell Regeneration
PI/PD, \$56,548
Total award: \$100,000

Merck & Company Inc. 03/12/2019 - 09/12/2019
Development of Computational Methods to Predict Peptide Aggregation
PI/PD
Total award: \$5,000

Internal Funding (sorted by end year)

Instructional Innovation Award, Purdue University 11/01/2016 – (Award Funds)
Virtual Reality Environment to Learn and Visualize Chemical Interactions
PI/PD
Total award: \$100,000

Purdue Research Foundation 06/01/2020 - 05/31/2021
Microglia as a target for Glioblastoma
PI/PD
Total award: \$31,119

Integrative Data Science Initiative, Purdue University 08/01/2018 - 08/09/2020
Engineering Data Science Algorithms
Multi-PI (Other PI: David Gleich)

Total award: \$234,000

Purdue Institute for Drug Discovery 09/01/2018 - 08/31/2020
New Inhibitors against Cancers harboring Secondary Kinase Mutations
Co-PI (PI: Herman Sintim, Purdue U.)
Total award: \$100,000

Ralph W. and Grace M. Showalter Trust 07/01/2019 - 06/30/2020
Immune Checkpoint Therapy for Epstein-Barr Virus (EBV) Associated Tumors
Co-PI (PI: Abdolmajid Kazemian, Purdue U.)
Total award: \$75,000

Purdue Research Foundation 06/01/2018 - 12/31/2019
Characterizing Microglial Phagocytosis Specificity for Target Identification in Neurodegenerative Disease
PI/PD
Total award: \$30,144

Ralph W. and Grace M. Showalter Trust 07/01/2017 – 06/30/2018
Multi-target Potent Synthetic Leads for Castration Resistant Prostate Cancer
PI/PD
Total award: \$75,000

Jim and Diann Robbers Cancer Award for New Investigators 05/18/2017 – 05/31/2018
Differential Nuclear Hormone Receptor Modulators to Combat Castration Resistant Prostate Cancer
PI/PD
Total award: \$30,000

Indiana Elks Association 11/18/2016 - 12/31/2017
Purdue University Center for Cancer Research
Multitarget Design & Synthesis of Potent Leads to Combat Castration Resistant Prostate Cancer
PI/PD
Total award: \$10,000

Before Purdue:

JDRF grant award 3-PDF-2014-205-A-N 2014-2016
Repurposing approved drugs as pancreatic beta cell survival therapies in type-1 diabetes
Role: PI/PD
Total award: \$169,872

Pending Proposals:

National Institutes of Health 06/01/2023 - 05/31/2028
1R01AG081444-01
Lipid Droplets induced Microglial Dysfunction in Alzheimer's Disease and Related Dementia
PI/PD
Total requested: \$4,014,947

National Science Foundation

09/01/2022 - 08/31/2025

Collaborative Research: MFB: Next-Generation Machine Learning Integrative Methods to enhance Biomolecular Nucleocytoplasmic Transport Strategies

Co-PI

Total requested: \$1,089,318

UES Inc.

09/01/2022 - 08/31/2023

Machine Learning (ML) based Damage Modeling of Polymer Matrix Composites

PI/PD

Total requested: \$60,000

Teledyne FLIR LLC

08/01/2022 - 04/30/2026

High Throughput Desorption Electrospray Ionization Mass Spectrometry (HT-DESI-MS) for Characterization of Biological Systems AIMS-HITS – Ambient Ionization Mass Spectrometry High Throughput Screening

Co-PI

Total requested: \$1,952,496

National Science Foundation

09/01/2022 - 08/31/2025

NSF Rational Engineering and Applications of Chemical Tenets (REACT) Science and Technology Center (STC)

Co-PI (co-Director of the Center)

Total requested: \$30,000,000

PUBLICATIONS**Journal Tier Evaluation**

Journal Name	Journal Abbreviation	Impact Factor	# of Papers (Independent)	# of Papers (Total)
Nature	<i>Nature</i>	42.78	1	1
Immunity	<i>Immunity</i>	22.55	1	2
Angewandte Chemie, International Edition	<i>Angew. Chem., Int. Ed.</i>	12.96	1	1
Journal of Clinical Investigation	<i>J. Clin. Investig.</i>	12.28		1
Nucleic Acids Research	<i>Nucleic Acids Res.</i>	11.50		1
Proceedings of National Academy of Sciences	<i>Proc. Natl. Acad. Sci. U. S. A.</i>	11.20		2
Chemical Science	<i>Chem. Sci.</i>	9.82	3	3
Cancer Research	<i>Cancer Res.</i>	9.13	1	1
Diabetes	<i>Diabetes</i>	7.72	1	1
Drug Discovery Today	<i>Drug. Discov. Today</i>	6.88	1	2
Organic Letters	<i>Org. Lett.</i>	6.55	1	1
Bioinformatics	<i>Bioinformatics</i>	5.61	1	1

Frontiers in Chemistry	<i>Front. Chem.</i>	5.22	1	1
Journal of Immunology	<i>J. Immunol.</i>	4.72		1
Scientific Reports	<i>Sci. Rep.</i>	4.57	2	2
Journal of Chemical Information and Modeling	<i>J. Chem. Inf. Mod.</i>	4.55	3	3
Advances in Dental Research	<i>Adv. Dent. Res.</i>	4.37		1
ACS Medicinal Chemistry Letters	<i>ACS Med Chem Lett.</i>	3.97	1	1
Future Medicinal Chemistry	<i>Future Med Chem.</i>	3.62	1	1
Molecules	<i>Molecules</i>	3.26	1	1
Chem Bio Chem	<i>ChemBioChem</i>	3.16	1	1
Mini Reviews in Medicinal Chemistry	<i>Mini Rev. Med. Chem.</i>	2.91		1
Proteins: Structure, Function, and Bioinformatics	<i>Proteins</i>	2.83		2
PLOS One	<i>PLoS One</i>	2.78		1
Current Pharmaceutical Design	<i>Curr. Pharm. Des</i>	2.57	1	1
Islets	<i>Islets</i>	2.48	1	1
Methods and Protocols	<i>Methods and Protocols</i>	1.84	1	1

Refereed (Total: 36; Independent: 24)

Corresponding author is denoted by (*), postdoc by (P), graduate students by (G), undergraduates by (U) and as a collaborator/co-author by (C). [Media mention or Paper Highlight](#). [IF = Impact Factor].

Independent Publications from Purdue:

1. Falls Z, Fine J^(G), Chopra G^(*), Samudrala R. Accurate prediction of inhibitor binding to HIV-1 protease using CANDOCK. *Front. Chem.* **9** (2022). DOI: <https://doi.org/10.3389/fchem.2021.775513> [IF=5.22]
2. Jethava KP^(P), Prakash P^(G), Manchanda P^(G), Arora H^(G), Chopra G^(*). One Scaffold – Different Organelles Sensors: pH-Activable Fluorescent Probes for Targeting Live Microglial Cell Organelles. *ChemBioChem.* **23**, 9, e202100378. (2022). DOI: <https://doi.org/10.1002/cbic.202100378>
Invited Front Cover: <https://doi.org/10.1002/cbic.202100667> [IF=3.16]
3. Guttenplan K, Weigel MK, Prakash P^(G), Wijewardhane PR^(G), Hasel P, Rufen-Blanchette U, Münch AE, Blum JA, Fine J^(G), Neal M, Bruce KD, Gitler AD, Chopra G, Liddel SA, Barres B. Neurotoxic reactive astrocytes induce cell death via saturated lipids. *Nature.* **599**, 102–107 (2021). DOI: <https://doi.org/10.1038/s41586-021-03960-y>. [IF=42.77]

4. Prakash P^(G), Jethava KP^(P), Korte N, Izquierdo P, Favuzzi E, Rose IVL, Guttenplan KA, Manchanda P^(G), Dutta S, Rochet J-C, Fishell G, Liddelow S, Attwell D, Chopra G^(*). Monitoring phagocytic uptake of amyloid- β into glial cell lysosomes in real-time. *Chem Sci.* **12**, 10901-10918 (2021) DOI: <https://doi.org/10.1039/D1SC03486C> [IF=9.82]

5. Arya CK, Yadav S, Fine JA^(G), Casanal A, Chopra G^(*), Ramanathan G, Vinothkumar KR, Subramanian R. A 2-Tyr-1-Carboxylate Mononuclear Iron Center is the Active Site of Dimethylformamidase. *Angew Chemie. Int. Ed.* **59**, 39, 16961-16966 (2020). DOI: <https://doi.org/10.1002/anie.202005332> [IF=12.96]

6. Fine JA^(G), Anand AR^(U), Jethava KP^(P), Chopra G^(*). Spectral deep learning for prediction and prospective validation of functional groups. *Chem. Sci.* **11**, 4618-4630 (2020). DOI: <https://doi.org/10.1039/C9SC06240H> *Chem Sci Pick of the Week* [IF=9.82]

7. Fine JA^(G), Li JK-Y, Beck A^(G), Alzarieni KZ, Ma X, Boulos V, Kenttämaa, HI, Chopra G^(*). Graph based machine learning interprets and predicts diagnostic isomer-selective ion-molecule reactions in tandem mass spectrometry. *Chem. Sci.* **11**, 11849-11858 (2020). DOI: <https://doi.org/10.1039/D0SC02530E> [IF=9.82]
<https://www.drugdiscoverynews.com/machine-learning-improves-tandem-ms-14906>
<https://phys.org/news/2020-10-machine-characterize-compounds-drug-discovery.html>
https://eurekaalert.org/pub_releases/2020-10/pu-mlm101320.php
<https://www.purdue.edu/newsroom/releases/2020/Q4/machine-learning-model-helps-characterize-compounds-for-drug-discovery.html>
<https://www.labmanager.com/news/machine-learning-model-helps-characterize-compounds-for-drug-discovery-24096>
<https://www.newsbreak.com/indiana/west-lafayette/news/2081767096332/machine-learning-model-helps-characterize-compounds-for-drug-discovery>

8. Jethava KP^(P), Fine JA^(G), Chen Y^(U), Hossain A^(G), Chopra G^(*). Accelerated reactivity mechanism and interpretable machine learning model of *N*-Sulfonylimines toward fast multicomponent reactions. *Org. Lett.* **22**, 21, 8480–8486 (2020). DOI: <https://doi.org/10.1021/acs.orglett.0c03083> [IF=6.55]
<https://www.drugdiscoverytrends.com/researchers-aim-to-speed-drug-discovery-with-human-understandable-ml-models/>
<https://www.purdue.edu/newsroom/releases/2020/Q4/one-step-multicomponent-reaction-with-interpretable-machine-learning-innovation-to-develop-chemical-library-for-drug-discovery.html>

9. Mangione W, Falls Z, Melendy T, Chopra G^(*), Samudrala R. Shotgun drug repurposing biotechnology to tackle epidemics and pandemics. *Drug Discov. Today.* **25**, 7, 1126-1128 (2020). DOI: <https://doi.org/10.1016/j.drudis.2020.05.002> [IF=6.88]

10. Fine JA^(G), Muhoberac M^(G), Fraux G, Chopra G^(*). DUBS: A framework for developing Directory of Useful Benchmarking Sets for virtual screening. *J. Chem. Inf. Model.* **60**, 9, 4137-4143 (2020). DOI: <https://doi.org/10.1021/acs.jcim.0c00122> [IF=4.55]

11. Mangione W, Falls Z, Chopra G^(C), Samudrala R. cando.py: Open source software for analyzing large scale drug-protein-disease data. *J. Chem. Inf. Model.* 60, 9, 4131-4136 (2020). DOI: <https://doi.org/10.1021/acs.jcim.0c00110> [IF=4.55]
Contribution: Developed the concepts and software modules for cando multitargeting framework
12. Robertson MA, Padgett LR, Fine JA, Chopra G^(C), Mastracci TL. Targeting polyamine biosynthesis to stimulate beta cell regeneration in zebrafish. *Islets.* Sep 2;12(5):99-107 (2020). DOI: <https://doi.org/10.1080/19382014.2020.1791530> [IF=2.48]
Contribution: Prediction of molecules tested for polyamine biosynthesis on which the publication is based
13. Fine JA^(G), Konc J, Samudrala R, Chopra G^(*). CANDOCK: Chemical atomic network based hierarchical flexible docking algorithm using generalized statistical potentials. *J. Chem. Inf. Model.* 60, 3, 1509-1527 (2020). DOI: <https://doi.org/10.1021/acs.jcim.9b00686> [IF=4.55]
14. Chakravorty S, Yan B, Wang C, Wang L, Quaid JT, Lin CF, Briggs SD, Majumder J^(P), Canaria DA, Chauss D, Chopra G^(C), Olson M, Zhao B, Afzali B, Kazemain M. Integrated pan-cancer map of EBV-associated neoplasms reveals functional host-virus interactions. *Cancer Res.* 79, 23, 6010-6023 (2019). DOI: <https://doi.org/10.1158/0008-5472.CAN-19-0615>. [IF=9.13]
Contribution: Identification of immune checkpoints PD-1/PD-L1 pathway verified in the manuscript
<https://medicalxpress.com/news/2019-10-gene-interactions-cancer-therapies.html>
<https://www.healthcanal.com/cancers/249184-map-showing-gene-interactions-could-lead-to-new-cancer-therapies.html>
15. Fine JA^(G), Lackner R, Samudrala R, Chopra G^(*). Computational chemoproteomics to understand the role of selected psychoactives in treating mental health indications. *Sci. Rep.*, 9:13155 (2019). [IF=4.57]
<https://www.medindia.net/news/drug-discovery-platform-may-provide-new-options-for-treating-mental-health-illnesses-190966-1.htm>
<https://www.technologynetworks.com/tn/news/platform-developed-to-help-find-treatments-for-mental-health-illnesses-325235>
<https://www.news-medical.net/news/20191015/CANDO-drug-discovery-platform-focuses-on-finding-new-medications-for-mental-illnesses.aspx>
https://www.greensburgdailynews.com/news/lifestyles/new-options-for-treating-mental-health-illnesses/article_6c18000e-2e5d-11ea-86b3-bbfc7afb880.html
<https://medicalxpress.com/news/2019-10-drug-discovery-platform-options-mental.html>
16. Fine JA^(G), Chopra G^(*). Lemon: a framework for rapidly mining structural information from the Protein Data Bank. doi: 10.1093/bioinformatics/btz178. *Bioinformatics*, 35(20):4165-67 (2019). [IF=5.61]
<https://weatherherald.com/drugs/lemon-machine-learning-create-drugs-0060082>
<https://healthitanalytics.com/news/data-mining-tool-could-help-train-machine-learning-models>
https://www.eurekalert.org/pub_releases/2019-12/pu-tc121919.php
<https://www.sciencedaily.com/releases/2019/12/191220074256.htm>
<https://scitechdaily.com/creating-better-drugs-with-this-lemon-for-machine-learning/>
<https://techxplore.com/news/2019-12-lemon-machine-drugs.html>
<https://insights.globalspec.com/article/13208/new-software-helps-create-better-drugs>
<https://indicanews.com/2019/12/23/gaurav-chopras-lemon-to-analyze-data-faster/>

17. Prakash P^(G), Lantz TC^(U), Jethava KP^(P), Chopra G^(*). Rapid, Refined, and Robust Method for Expression, Purification, and Characterization of Recombinant Human Amyloid-beta 1-42. *Methods and Protocols*, 2(2), 48. (2019).
<https://www.alzforum.org/papers/rapid-refined-and-robust-method-expression-purification-and-characterization-recombinant>
18. Keasar C, McGuffin LJ, Wallner B, Chopra G^(C), *et. al.* An analysis and evaluation of the WeFold collaborative for protein structure in CASP11 and CASP12. *Sci. Rep.*, 8, 9939 (2018). [IF=4.57]
Contribution: Development of methods and modules for protein structure refinement.
19. Hernandez-Perez M, Chopra G^(C), Fine J^(G), Anderson RM, Benjamin C, Nadler JL, Holman TR, Maloney DJ, Tersey SA, Mirmira RG. Inhibition of 12/15-lipoxygenase protects against β cell oxidative stress and glycemic deterioration in mouse models of type 1 diabetes. *Diabetes*, 66 (11), 2875-2887 (2017). [IF=7.72]
Contribution: Proteome-scale modeling to identify toxicity and 12/15-lipoxygenase interaction modeling of small molecules validated by experiments done in the manuscript.
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23. Esensten JH, Helou YA, Chopra G^(C), Weiss A, Bluestone JA. CD28 costimulation: from mechanism to therapy. *Immunity* 44(5): 973-988 (2016). [IF=22.55]
24. Chopra G^(*), Samudrala R. Exploring polypharmacology in drug discovery and repurposing using the CANDO platform. *Current Pharm. Des.* 22(21): 3109-3123 (2016). [IF=2.57]

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<https://www.ncbi.nlm.nih.gov/pubmed/25692693>
28. Ali ZA, de Jesus Perez V, Yuan K, Orcholski M, Pan S, Qi W, Chopra G, Adams C, Kojima Y, Leeper NJ, Qu X, Zaleta-Rivera K, Kato K, Yamada Y, Oguri M, Kuchinsky A, Channon K, Charest A, Quertermous T, Ashley EA. Oxido-reductive regulation of human vascular remodeling by the orphan receptor tyrosine kinase ROS1. *J. Clinical Investigation* 124(12): 5159-74 (2014). [IF=12.28]
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29. Chopra G[#], Minie ME[#], Sethi G[#], Horst JA[#], Roy A, White G, Samudrala R. CANDO and the infinite drug discovery frontier. *Drug Discov. Today* 19(9):1353-63 (2014). [#]Contributed equally [IF=6.88]
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31. Lertkiatmongkol P, Assawamakin A, White G, Chopra G, Rongnoparut P, Samudrala R, Tongsimma S. Distal effect of amino acid substitutions in CYP2C9 polymorphic variants causes differences in interatomic interactions against (S)-warfarin. *PLoS One* 8(9): e74053 (2013). [IF=2.78]
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33. Rodrigues J, Levitt M and Chopra G^(*). KOBAMIN – KnOwledge BAsed MINimization server for protein structure refinement. *Nucleic Acid Research, Web Server Issue*. 40 (W1): W323-W328 (2012). [IF=11.50]
34. Chopra G^(*) and Levitt M. Remarkable patterns of surface water ordering around polarized buckminsterfullerene. *Proc. Natl. Acad. Sci. U.S.A.* 108(35):14455-14460 (2011). [IF=11.20]
<https://phys.org/news/2011-08-polarization-affects-h2o-revealed-molecular.html>
35. Chopra G^(*), Kalisman N & Levitt M. Consistent refinement of submitted models at CASP using a knowledge-based potential. *Proteins* 78(12): 2668-2678 (2010). [IF=2.5]
36. Chopra G, Summa CM & Levitt M. Solvent dramatically affects protein structure refinement. *Proc. Natl. Acad. Sci. U.S.A.* 105(51): 20239-20244 (2008). [IF=11.20]

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37. Evans BR, Yeung L, Beck AG^(G), Li A, Lee DH, Chopra G^(*), Bateman KP. Automated Bioanalytical Workflow for Ligand Binding based Pharmacokinetic Assay Development. *Analytical Chemistry*. Major Revision 2022.
 chemRxiv [Preprint]. Available from (doi): <https://doi.org/10.26434/chemrxiv-2022-b3gn1>

38. Fine JA^(G), Dhawan D, Utturkar S, San Miguel P, Chopra G^(C), Turek J, Nolte D, Childress MO, Lanman NA. Integration of Biodynamic Imaging and RNA-seq predicts chemotherapy response in canine diffuse large B-cell lymphoma. bioRxiv 290353 [**Preprint**]. Available from (doi): <https://doi.org/10.1101/2020.09.11.290353>
Contribution: My graduate student is the lead author for this study; Supervised machine learning methods.
39. Wijewardhane PR^(G), Jethava KP^(P), Fine JA^(G), Chopra G^(*). Graph neural networks bootstrapped for synthetic selection and validation of small molecule immunomodulators. chemRxiv [**Preprint**]. Available from (doi): <https://doi.org/10.33774/chemrxiv-2021-r4xnx-v2>
40. Zhang W^(U), Fine JA^(G), Sculley C^(U), McGraw J, Chopra G^(*). Molecular Interactions using New Technology: A virtual reality gaming platform to visualize and manipulate molecules. chemRxiv 9889994 [**Preprint**]. Available from (doi): [10.26434/chemrxiv.9889994.v1](https://doi.org/10.26434/chemrxiv.9889994.v1)
41. Hossain A^(G), Majumder J^(P), Bi C, Huang F, Chopra G^(*). Stable and Reversible Functionalization and Super-Resolution Microscopy of Live Cell Membranes. bioRxiv 462044 [**Preprint**]. Available from (doi): <https://doi.org/10.1101/462044>
42. Fine JA^(G), Wijewardhane PR^(G), Mohideen Beer SD^(G), Smith K, Bothe J, Krishnamachari Y, Andrews A, Wuelfing P, Liu Y, Chopra G^(*). Learning relationships between chemical and physical stability for drug development. chemRxiv [**Preprint**]. Available from (doi): <https://doi.org/10.33774/chemrxiv-2021-r4xnx-v2>
43. Randolph CE^(P), Beveridge CH^(G), Iyer S^(G), Blanksby SJ, McLuckey SA, Chopra G^(*). Identification of monomethyl branched chain lipids by a combination of liquid chromatography tandem mass spectrometry and charge-switching chemistries. *Journal of the American Society for Mass Spectrometry*. Minor revision. 2022. chemRxiv [**Preprint**]. Available from (doi): <https://doi.org/10.26434/chemrxiv-2022-nrsv7>
44. Prakash P^(G), Manchanda P^(G), Paouri E, Bisht K^(P), Sharma K^(P), Wijewardhane PR^(G), Randolph CE^(P), Clark MG, Fine JA^(G), Thayer EA^(U), Prayson RA, Zhang C, Davalos D, Chopra G^(*). Amyloid β Induces Lipid Droplet-Mediated Microglial Dysfunction in Alzheimer's Disease. *Nature*. Submitted. 2022.

REFREED PUBLISHED ABSTRACTS AND NON-REFREED PUBLICATIONS

1. Chakravorty S, Yan B, Chauss D, Wang L, Canaria DA, Jethava K^(P), Chopra G^(C), Briggs SD, Zhao B, Olson MR, Afzali B, Kazemian M. The role of Virostatic genes in modulating Immune Checkpoints in Epstein-Barr Virus associated Tumors. *J Immunol* May 1, 2020, 204 (1 Supplement) 249.9.
2. Thayer EA^(U), Prakash P^(G), Fine JA^(G), Ferreira CR, Chopra G^(*). Lipidomic profiling in amyloid beta treated BV2 microglia. *4th Annual ECI Undergraduate Research Conference*, November 16th, 2019; University of Illinois Urbana-Champaign, Champaign, IL. (*presented by undergraduate student*)
3. Thayer EA^(U), Prakash P^(G), Chopra G^(*). Amyloid-beta mediated inflammatory response in microglia. *Summer Undergraduate Research Fellowship (SURF) Symposium*. (August 2019).

4. Kischuk E, Majumder J^(P), Fine JA^(G), Lantz TC^(U), Dhawan D, Knapp DW, Ratliff TL, Chopra G^(*). Cell-specific gene program-based small-molecule immunomodulators targeting solid-tumor microenvironments. *Cancer Research* 78 (13 Supplement), 4709-4709, (2018).
5. Majumder J^(P), Fine JA^(G), Lantz TC^(U), Conder CJ^(G), Chopra G^(*). Cancer cell specific lethality by degrading specific protein target network identified using a chemical screening based machine learning method. *Cancer Research* 78 (13 Supplement), LB-076-LB-076, (2018).
6. Kischuk E, Majumder J^(P), Fine JA^(G), Lantz TC^(U), Ratliff TL, Chopra G^(*). Chemical screening based machine learning platform to identify MDSC-specific gene programs and immunomodulators to target solid tumor microenvironments. *J Immunol* May 1, 2018, 200 (1 Supplement) 174.27.
7. Myoung S, Savinov S, Chen L, Chopra G^(C), Avramova L, Welch J, Loren B, Thompson D, Kasinski AL. Development of an RNA-based cancer therapeutic targeting the let-7-LIN28 interaction. *Cancer Research* 78 (13 Supplement), 4656-4656, (2018).
8. Thayer EA^(U), Prakash P^(G), Chopra G^(*). Role of cyclic GMP-AMP Synthase (cGAS) in Microglial Immune Response. *3rd Annual ECI Undergraduate Research Conference*, November 17th, 2018; University of Illinois Urbana Champaign, Champaign, IL. (*presented by undergraduate student*)
9. Williams GC^(U), Prakash P^(G), and Chopra G^(*). Targeting pro-inflammatory function of microglia using small molecules to combat neurodegeneration. *Summer Undergraduate Research Fellowship (SURF) Symposium*. Paper 100 (2018). (*presented by undergraduate student*)
10. Chopra G^(*). Targeting Proteome-Scale Networks to Design and Synthesize Potent Anticancer and Cell-Specific Immunomodulatory Compounds. *Biophysical Journal*, Volume 114, Issue 3, Supplement 1, p663a, 2 February 2018. DOI: <https://doi.org/10.1016/j.bpj.2017.11.3577>.
11. Majumder J^(P), Chopra G^(*). Live Cell Surface Conjugation Methods for Imaging, Sensing and Therapy. *Biophysical Journal*, Volume 114, Issue 3, Supplement 1, p20a, 2 February 2018. DOI: <https://doi.org/10.1016/j.bpj.2017.11.154>.
12. Fine J^(G), Chopra G^(*). CANDOCK: Conformational Entropy Driven Analytics for Class-Specific Proteome-Wide Docking. *Biophysical Journal*, Volume 114, Issue 3, Supplement 1, p57a, 2 February 2018. DOI: <https://doi.org/10.1016/j.bpj.2017.11.363>.
13. McGraw J, Zhang W^(U), Luginbuhl AD, Takahashi G, Tasker RF, Chopra G^(*). Virtual Reality Environment to Visualize and Manipulate Molecular Structures. *Biophysical Journal*, Volume 114, Issue 3, Supplement 1, p184a, 2 February 2018. DOI: <https://doi.org/10.1016/j.bpj.2017.11.1029>.
14. Majumder J^(P), Lantz TC^(U), Fine J^(G), Chopra G^(*). Drug repurposing for castration resistant prostate cancer based on disease-disease relationships [abstract]. In: Proceedings of the AACR Special Conference on Translational Control of Cancer: A New Frontier in Cancer Biology and Therapy; 2016 Oct 27-30; San Francisco, CA. Philadelphia (PA): *AACR, Cancer Res*, 77(6 Suppl): Abstract nr A35 (2017).
15. Lantz TC^(U), Majumder J^(P), and Chopra G^(*). Computational Drug Design: A Multitargeted Approach in Bladder Cancer. *Summer Undergraduate Research Fellowship (SURF) Symposium*. Paper 133 (2017). (*presented by undergraduate student*)
16. Stewart B^(U), Fine J^(G), Chopra G^(*). Parallelization of Molecular Docking algorithms using CUDA for use in Drug Discovery. *Summer Undergraduate Research Fellowship (SURF) Symposium*. Paper 136 (2017). (*presented by undergraduate student*)

17. Xu D, Dong S, Martínez-Llordella M, Chopra G^(C), Bluestone JA. Unveiling the specificity of islet-antigen specific regulatory T cells in T1D patient using single cell deep-sequencing. *Journal of Immunology* 196 (1 Supplement), 54.29-54.29 (2016).

PLENARY TALKS AND INVITED LECTURES

88 invitations, 2 Plenary talks, 2 Invited Workshop

Invitations since starting at Purdue: (59 invitations including 1 Plenary Talk and 3 Honorariums)

88. 6th International Conference on Mathematical and Computational Medicine, Telluride, CO, 11-15 June 2022
87. Invited Talk, Midwestern Thermodynamics and Statistical Mechanics, 6-7 June 2022
86. Invited Seminar, National Institute of Immunology, New Delhi, India, 25 May 2022
85. Invited Seminar, Regional Center for Biotechnology, Faridabad, Haryana, India, 24 May 2022
84. Neuroscience Seminar, Lerner Research Institute, Cleveland Clinic, Cleveland, OH, 27th April 2022
83. ACS President Initiative on Machine Learning, San Diego, 19th March 2022
82. Jacobs School of Medicine and Biomedical Sciences, University at Buffalo, Buffalo, NY, 4th August 2021
81. Department of Chemical Engineering, Massachusetts Institute of Technology (MIT), Cambridge, MA, 9th April 2021
80. Chemistry and Biochemistry Department, George Mason University, Fairfax, VA, 26th March 2021
79. Biology of Neurodegeneration (BOND) Seminar Series, School of Medicine, Oregon Health & Science University, Portland, OR, 12th March 2021
78. Department of Chemistry, Stanford University, Stanford, CA, 9th March 2021
77. Division of Chemistry and Chemical Engineering, California Institute of Technology (Caltech), Pasadena, CA, 2nd March 2021
76. Department of Chemistry & Biochemistry, University of Maryland, College Park, MD, 24th February 2021
75. Cancer Center at Illinois, University of Illinois at Urbana Champaign, Urbana, IL, 19th November 2020
74. Pacific Chem 2020: A Creative Vision for the Future, Honolulu, HI, December 2020 (*cancelled due to covid-19*)
73. Gordon Research Conference on Molecular Structure Elucidation, Newry, ME, August 2020 (*cancelled due to covid-19*)
72. 5th International Conference on Mathematical and Computational Medicine, Telluride Science Research Center, Telluride, CO, June 2020 (*cancelled due to covid-19*)
71. American Society of Mass Spectrometry (ASMS), Houston, TX, June 2020 (changed to *virtual*)
70. Mass Spectrometry Applications in Clinical Laboratory (MSACL), Palm Springs, CA, March 2020 (*cancelled due to covid-19*)
69. ACS National Meeting, Spring 2020, Philadelphia, PA, March 2020 (*cancelled due to covid-19*)

68. Department Colloquium, Chemistry and Chemical Biology, Rutgers University at New Brunswick, NJ, March 2020
67. Machine Learning in Analytical Chemistry, Pittcon 2020, Chicago, IL, March 2020
66. Purdue Institute for Integrative Neuroscience, Purdue University, West Lafayette, IN, December 2019
65. Materials Research Society Annual Meeting, Boston, MA, December 2019
64. NSF MolSSI Machine Learning in Chemistry, University of Maryland, College Park, MD, October 2019
63. IU/PU Traumatic Brain Injury Symposium, Indiana University School of Medicine, Indianapolis, IN, October 2019
62. *Plenary Talk*, SCIX 2019, Palm Springs, CA, October 2019
61. Institute of Immunology, University of California, Irvine, CA, October 2019
60. Stark Neuroscience Center, Indiana University School of Medicine, Indianapolis, IN, September 2019
59. Nationwide Children's Hospital Research Institute, Columbus, OH, June 2019
58. Great Lakes Regional ACS Meeting (Biologically Related Molecules & Processes), Lisle, IL, May 2019
57. Data Science Invited Talk Series, Indiana University School of Informatics, Computing and Engineering, Bloomington, IN, April 2019
56. Foundations of Data Science Conference, Purdue University, West Lafayette, IN, April 2019
55. Pharmaceutical Sciences Seminar and *Honorarium*, Merck & Company, Rahway, NJ, December 2018
54. Discussion Leader and Speaker, Gordon Research Conference on Molecular Structure Elucidation, Newry, ME, August 2018
53. Department of Cancer Genetics and Genomics, Roswell Park, Buffalo, NY, June 2018
52. 4th Midwest Tumor Microenvironment Meeting, Iowa City, IA, May 2018
51. ACS National Meeting, Spring 2018, New Orleans, LA, March 2018
50. Virtual Reality and Healthcare Symposium, Harvard University, Boston, MA, March 2018
49. Future of the Chemical Sciences Symposium, Chicago, IL, December 2017
48. PI4D Mini Symposium on Frontiers of Immunology, West Lafayette, IN, October 2017
47. Purdue Institute for Drug Discovery Symposium, West Lafayette, IN, October 2017
46. Institute Seminar and *Honorarium*, National Center for Biological Sciences (NCBS), Bangalore, India, August 2017
45. 25th Annual International Conference on Intelligent Systems for Molecular Biology (ISMB 2017), Prague, Czech Republic (3DSig meeting), July 2017
44. Department of Pharmacology, University of California, Davis, CA, March 2017
43. Department of Medicinal and Biological Chemistry, University of Toledo, OH, November 2016
42. Walther Cancer Foundation Inc. Annual Symposium, Lafayette, IN, November 2016
41. Purdue Institute for Drug Discovery Symposium, West Lafayette, IN, September 2016

40. Purdue Center for Cancer Research, West Lafayette, IN, August 2016
39. Grand Rounds Seminar and *Honorarium*, Eli Lilly and Company, Indianapolis, IN, July 2016
38. 24th Annual International Conference on Intelligent Systems for Molecular Biology (ISMB 2016), Orlando, FL, July 2016
37. Neuronetworking Series, Purdue Institute for Integrative Neuroscience, West Lafayette, IN, June 2016
36. NSF ‘Research goes to school’ – Talk for High School Teachers, West Lafayette, IN, June 2016
35. Oden Institute for Computational Engineering & Sciences, The University of Texas at Austin, Austin, TX, May 2016
34. Lawrence Livermore National Lab Day, Purdue Center for Cancer Research, May 2016
33. 3rd International Conference on Mathematical and Computational Medicine, Nationwide Children’s Hospital, Columbus, OH, May 2016
32. Center for Diabetes and Metabolic Diseases, IU School of Medicine, Indianapolis, IN, April 2016
31. Big Data Seminar, Statistics Department, Purdue University, West Lafayette, IN, February 2016
30. Physical Chemistry Seminar, Purdue University, West Lafayette, IN, February 2016

Invitations before Purdue: (29 invitations)

29. 23rd Annual International Conference on Intelligent Systems for Molecular Biology (ISMB 2015), Dublin, Ireland, July 2015
28. Department of Pharmaceutical Sciences, University of Colorado – Anschutz Medical Campus, Denver, CO, April 2015
27. Department of Chemistry, College of Science, Purdue University, West Lafayette, IN, March 2015
26. 2nd Zing Mathematical & Computational Medicine Conference, Cancun, Mexico, December 2014
25. Diabetes Center, University of California, San Francisco, CA, September 2014
24. Protein Folding Conference, Punta Cana, Dominican Republic, July 2014
23. 22nd Annual International Conference on Intelligent Systems for Molecular Biology (ISMB 2014), Boston, MA, July 2014
22. *Panelist*, Honoring Michael Levitt’s Nobel Prize, ISMB 2014 Conference, Boston, MA, July 2014
21. Department of Biological Sciences, Florida Gulf Coast University, Ft. Myers, FL, June 2013
20. Laboratory of Molecular Biology, Medical Research Council, Cambridge, UK, December 2012
19. 10th Critical Assessment of Techniques for Protein Structure Prediction, Gaeta, Italy, December 2012
18. Chemistry Department, Hong Kong University of Science & Technology, Hong Kong, October 2012
17. Biomolecular Modeling & Design, Bioinformatics Institute, A*STAR, Singapore, October 2012
16. *Plenary Talk*, International Conference on Bioinformatics (InCoB 2012), Thailand, October 2012
15. Multiscale Modeling Workshop, InCoB 2012, Thailand, October 2012
14. Aug 2012 - Bluestone Group Meeting, University of California, San Francisco, CA
13. July 2012 - Joseph DeRisi’s Group Meeting, University of California, San Francisco, CA

12. Multiresolution Molecular Modeling workshop, Uppsala University, Sweden, June 2011
11. Mar 2011 - Hana El-Samad's Group Meeting, University of California, San Francisco, CA
10. Department of Chemistry, University of Pacific, Stockton, CA, February 2011
9. 9th Critical Assessment of Techniques for Protein Structure Prediction, Asilomar, CA, December 2010
8. High Performance Computing Day, Stanford University, Stanford, CA, August 2010
7. CoCrystal Pharma Inc., Mountain View, CA, December 2009
6. Biomedical Computation at Stanford (BCATS), Stanford, CA, November 2009
5. 8th Critical Assessment of Techniques for Protein Structure Prediction, Sardinia, Italy, December 2008
4. Department of Chemistry, Indian Institute of Technology - Delhi, New Delhi, India, April 2008
3. Center for Protein Folding Machinery Nanomedicine Retreat, Stanford, CA, May 2007
2. Critical Assessment of Prediction of Interactions (CAPRI), 3rd Meeting, Toronto, Canada, April 2007
1. International Conference on Bioinformatics (InCoB), New Delhi, India, December 2006

OTHER PRESENTED PAPERS

At Purdue:

39. **SfN Neuroscience 2022**, San Diego, CA, November 12-16, 2022
Amyloid β Induces Lipid Droplets in Microglia Leading to their Phagocytic Dysfunction (Talk)
38. **ACS Annual Meeting and Expo**, Chicago, IL, August 21-25, 2022
 - a. *Paddy: Evolutionary algorithm for chemical systems and spaces (Talk - Computers in Chemistry Division)*
 - b. *Structure-organelle-relationship (SOR) of pH-activable fluorescent probes for targeting live microglial cell organelles (Talk - Biological Chemistry Division)*
 - c. *Stable and reversible functionalization and super-resolution microscopy of live cell membranes (Talk - Biological Chemistry Division)*
 - d. *Neural networks to predict peptide formulation stability (Talk - Chemical Information Division)*
 - e. *Cliquify: Robust representation of molecular graphs to trees structures (Poster - Computers in Chemistry Division)*
 - f. *pH-Responsive chemical tools for glial cells (Poster - Analytical Chemistry Division)*
37. **Gordon Research Conference on Lipidomics and Decoding Life: From the Technology and Biology Landscapes to Clinical Adaptation**, Newry, ME, August 7-12, 2022
Lipid Structural Profiles of Microglia in Alzheimer's Disease using LC-MS/MS OzESI-MRMs (Poster)
36. **Glia in Health and Disease**, Cold Spring Harbor Laboratory, NY, July 21-25, 2022
Amyloid β Induces Lipid Droplets in Microglia Leading to their Phagocytic Dysfunction (Poster)
Impact Induces Phagocytic Defect in Reactive Microglia (Poster)
Injury Induces Lipid-Droplet Accumulation in Microglia Coupled with Phagocytic Defects (Poster)
35. **ASMS Conference on Mass Spectrometry and Allied Topics**, Minneapolis, MN, Jun 5-9, 2022

- a. *Development of Detailed Lipid Structural Profiles of Microglia in Alzheimer's Disease (Talk)*
 - b. *Machine Learning Framework for Accurate Prediction of Functional Groups from Tandem Mass Spectrometry Experiments (Talk)*
 - c. *Machine Learning Guided Automated HPLC/MS/MS Platform Based on Diagnostic Ion-molecule Reactions for Structural Identification of Unknown Compounds (Talk)*
 - d. *Isomer-resolved quantitative imaging of lipids reveals variations in isomeric abundance in an Alzheimer's mouse model (Poster)*
 - e. *Mass spectrometry imaging of lipidome in a mouse model of Alzheimer's disease (Poster)*
34. **ACS Annual Meeting and Expo**, San Diego, CA, March 20 - 24, 2022
SMART: Single Molecule fluorescent Activation in Real Time for molecular computations and sensing (Poster)
33. **Neuroscience 2021**, Society for Neuroscience Annual Meeting, Chicago, IL, Nov 8-11, 2021 (virtual); Nov 13-16, 2021 (in-person)
Injury induced lipid droplet associated microglia with defective phagocytosis (Poster)
32. **ASMS Conference on Mass Spectrometry and Allied Topics**, Philadelphia, PA, Oct 31-Nov 4, 2021
Charge switching chemistries for the structural elucidation of methyl branched lipids (Poster)
31. **ACS Annual Meeting and Expo**, August 22 - 26, 2021, Atlanta, GA
Automating optimization of experimental parameters for pulsed introduction of neutral reagents in tandem mass spectrometry experiments based on diagnostic gas phase ion-molecule reactions (Live Session – Machine Learning and Automation in Chemistry – ANYL, COMP, CINF division)
30. **ACS Annual Meeting and Expo**, April 5 - 30, 2021 (virtual)
- a. *Guiding chemical reactions in different environments using interpretable machine learning models (Live Session – Chemical Information CINF division)*
 - b. *Local and global feature-based graph neural networks bootstrapped for synthetic selection of small molecule immunomodulators (Live Session – Computers in Chemistry COMP division)*
29. **260th ACS Annual Meeting and Expo**, San Francisco, CA, Aug 17 - Aug 22, 2020 (virtual)
- a. *Machine learning for analytical chemistry using traditional and deep learning techniques: advancements and outlook (Broadcast – Analytical Chemistry ANYL division)*
 - b. *Docking-based graph neural networks for synthesis selection and experimental validation of potent PDI/PD-L1 inhibitor scaffolds (Broadcast – Computers in Chemistry COMP division)*
 - c. *Computational chemoproteomics to understand the role of psychoactives in treating mental health indications (Broadcast – Computers in Chemistry COMP division)*
 - d. *Is web assembly the future of visualizing molecules in the browser? (Broadcast – Chemical Information CINF division)*
 - e. *Big data driven solvent selection via deep learning to facilitate the discovery of green synthetic methodology (On-demand Oral – Organic Chemistry ORGN division)*
 - f. *Accelerated reactivity mechanism and interpretable machine learning model of N-sulfonylimines towards fast multicomponent reactions (On-demand Oral – Organic Chemistry ORGN division)*
 - g. *Lemon: Framework for rapidly mining structural information from the Protein Data Bank (Poster – Computers in Chemistry COMP division)*

28. **Glia in Health and Disease**, Cold Spring Harbor Laboratory, NY, July 16-19, 2020 (*virtual*)
- What do microglia make when they eat amyloid β ? (Talk)*
 - Do primary mouse microglia live a good life in culture? (Poster)*
27. **ASMS Conference on Mass Spectrometry and Allied Topics**, Houston, TX, May 31-June 4, 2020 (*virtual*)
- Graph-based machine learning interprets and predicts diagnostic isomer-selective ion-molecule reactions in tandem mass spectrometry (Talk)*
 - Multiple-Reaction Monitoring (MRM)-Profiling reveals distinct lipid and metabolite profiles in microglia with amyloid beta exposure (Poster)*
26. **259th ACS Annual Meeting and Expo**, Philadelphia, PA, Mar 22-Mar 26, 2020 (*canceled due to covid-19*)
- Big data driven solvent selection via deep learning to facilitate the discovery of green synthetic methodology*
 - Docking-based graph neural networks for synthesis selection and experimental validation of potent PDI/PD-L1 inhibitor scaffolds*
 - Computational chemoproteomics to understand the role of psychoactives in treating mental health indications*
 - Lemon: Framework for rapidly mining structural information from the Protein Data Bank*
25. **Indiana Clinical and Translational Sciences Institute (CTSI) Annual Meeting**, Indianapolis, IN, Sept 13, 2019
- Identifying molecular modulators of amyloid beta phagocytosis*
24. **Annual Meeting of Greater Indiana Society for Neuroscience**, Indianapolis, IN, Mar 22, 2019
- Characterizing microglial phagocytosis with novel pH-sensitive fluorescent amyloid- β sensor and α -synuclein sensors.*
23. **12th Annual Midwest Islet Club, University of Michigan**, Ann Arbor, MI, May 19-20, 2019
- Islet Conjugation for Local Immune Modulation During Transplantation.*
22. **Indiana Life Sciences Summit**, Indianapolis, IN, Oct 9-10, 2018
- Molecular interactions using new technologies (MINT) to gamify drug design.*
21. **19th International Conference on Alzheimer's Drug Discovery**, Jersey City, NJ, Sept 17-18, 2018
- A pH-Dependent Fluorogenic Amyloid-Beta Reporter for the Characterization of Phagocytosis in Live Microglial Cells: Implications for Alzheimer's Disease Research.*
20. **Molecular Structure Elucidation Gordon Research Conference**, Newry ME, August 12 - 17, 2018
- Machine Learning Based Integration of Proteome-Scale Interaction Modeling and Phenotypic Experiments to Design Small Molecules Drugs.*
19. **Glia in Health and Disease**, Cold Spring Harbor Laboratory, NY, July 19-23, 2018
- Do activated microglia get "exhausted" resulting in loss of function?: Development of pH-dependent fluorescent amyloid- β and α -synuclein sensors to study microglial phagocytosis*
18. **257th ACS Annual Meeting and Expo**, Orlando, FL, Mar 31-Apr 4, 2019
- Machine learning architectures to enhance chemical functional group predictions*

- b. *Neural networks incorporating entropy and machine learning improved crystal pose predictions and affinity ranking of small molecules*
 - c. *Machine learning based integration of proteome-scale interaction modeling and phenotypic experiments to design small molecule drugs*
 - d. *Synthetically facile stable and reversible cell-surface functionalization for cell based therapeutic applications*
17. **4th Midwest Tumor Microenvironment Meeting**, Iowa City, IA, May 21-23, 2018
MDSC specific gene program based small molecule immunomodulators targeting solid tumor microenvironments.
16. **Immunology 2018, AAI Annual Meeting**, Austin, TX, May 4-8, 2018
Chemical screening-based machine learning platform to identify MDSC-specific gene programs and immunomodulators to target solid tumor microenvironments.
15. **AACR Annual Meeting**, Chicago, IL, Apr 14-18, 2018
- a. *Cancer cell specific lethality by degrading specific protein target network identified using a chemical screening-based machine learning method.*
 - b. *Cell-specific gene program-based small-molecule immunomodulators targeting solid-tumor microenvironments.*
14. **255th ACS Annual Meeting and Expo**, New Orleans, LA, Mar 18-22, 2018
- a. *Live cell surface conjugation methods for imaging and sensing*
 - b. *Virtual reality environment to visualize and manipulate chemical interactions*
 - c. *Cell-specific chemical libraries targeting immune suppression in the tumor microenvironment*
13. **Virtual Reality and Healthcare Symposium**, Harvard Medical School, Boston, MA, Mar 4-6, 2018
Molecular trekking for drug discovery using MINT virtual reality platform.
12. **62nd Biophysical Society Annual Meeting**, San Francisco, CA, Feb 17-21, 2018
- a. *CANDOCK: Conformational entropy driven Analytics for class-specific proteome-wide DOCKing.*
 - b. *Targeting proteome-scale networks to design and synthesize potent anticancer and cell-specific immunomodulatory compounds.*
 - c. *Virtual reality environment to visualize and manipulate molecular structures.*
11. **Lymphocytes and their Roles in Cancer Keystone meeting**, Keystone, CO, Feb 11-15, 2018
Cell-specific small molecule immunomodulator targeting the tumor microenvironment in bladder cancer.
10. **Neuroinflammation: Concepts, Characteristics, Consequences**, Keystone, CO, 2017
Combination drug repurposing for synergistic effect of enhancing phagocytosis and reduce neurotoxicity during neurodegeneration based on disease-disease relationships
9. **Frontiers in Cancer Immunotherapy**, New York, NY, 2017
Dual action potent anticancer small molecule immunotherapeutic antagonizing immunosuppression in the tumour microenvironment
8. **61st Annual Biophysical Society Meeting**, New Orleans, LO, 2017

Interactome based drug discovery, design & disease-disease relationships

7. **AACR Translational Control**, San Francisco, CA, 2016
Drug repurposing for castration resistant prostate cancer using disease-disease relationships

Before Purdue:

6. **UCSF Diabetes Center Symposium**, Santa Cruz, CA, 2014
Multitargeting to prevent and reverse autoimmune diabetes in NOD mice
5. **TNF2013 Conference**, Quebec City, Canada, 2013
Predicting TNF- α pathway interactomics using a protein docking algorithm (presented by high school student)
4. **NIH Director's Pioneer Award Symposium**, Bethesda, Maryland, 2011
Computational Analysis of Novel Drug Opportunities
3. **22nd Protein Society Meeting**, San Diego, CA, 2008
Simulations in Solvent Dramatically Affect Protein Structure Refinement
2. **International Conference on Bioinformatics**, New Delhi, India, 2006
Stability of short aromatic-rich peptide segments in hydrophobic collapse
1. 2006 **Biomedical Computation at Stanford (BCATS) Conference**, Stanford, CA, 2006
Protein Denaturation in Nanodroplet

PATENTS AND DISCLOSURES

(Composition of matter)

- *Modifying surface of a live cell and the uses thereof*. Application #: 62658638, EFS ID: 32356462, 35750371. <https://inventions.prf.org/innovation/6812> ; Provisional Patent Application filed – 17 Apr 2018; International PCT application filed – 17 Apr 2019 – PCT/US19/27808; National Patent Application filed – 16 Oct 2020. **U.S. Patent/PCT Publication Number: WO/2019/204392**. <https://patents.google.com/patent/WO2019204392A1/> U.S. Patent Application Number: 17/048,340. <https://uspto.report/patent/app/20210148918>
- *Compounds for targeted therapies of Castration Resistant Prostate Cancer*. Application #: 62811747, EFS ID: 35284329. <https://inventions.prf.org/innovation/7139>; Provisional Patent Application filed – 28 Feb 2019; International PCT application filed – 28 Feb 2020 - PCT/US20/20332. **U.S. Patent/PCT Publication Number: WO 2020/176843**
- *pH-dependent composition matters useful for study and diagnosis of Alzheimer's disease*. Application #: 62826526, EFS ID: 35577854, 38986374; Attorney Docket No. 68541-02; <https://inventions.prf.org/innovation/7145>; Provisional Patent Application filed – 29 Mar 2019; International PCT application filed – 27 Mar 2020 – PCT/US20/25113. **U.S. Patent/PCT Publication Number: WO 2020/205465**
- *Compounds with immunomodulatory activity and uses thereof*. Application #: 62987914, EFS ID: 38829459, 42097540; Attorney Docket No. 68949-02; <https://inventions.prf.org/innovation/7559>;

Provisional Patent Application filed – 11 Mar 2020; International PCT application filed – 5 Mar 2021 – PCT/US21/20992.

- *pH-Activable Fluorescent Probes for Targeting Cell Organelles*. Application #: 63160201, EFS ID: 42167545; Attorney Docket No. 69413-01; <https://inventions.prf.org/innovation/8024>; Provisional Patent Application filed – 12 Mar 2021.

PROFESSIONAL ACTIVITIES

Grant Reviewer.

National Institutes of Health. CSR ZRG1 ETTN-J (02): Bioengineering, Cellular and Circuit Neuroscience

National Institutes of Health. CSR ETTN13: Neuroscience Assay, Diagnostics and Animal Model Development

Scientific Meetings Organized/Chaired

Nanosymposium, Neuroscience 2022, San Diego, CA
Chair, Microglial Activity and Dysfunction Session
November 2022, Society of Neuroscience Annual Meeting

Gordon Research Conference, Molecular Structure Elucidation, Newry ME
2024, 2022, 2020 Vice-chair
2018 Discussion Leader (*Session*: Advancing Pharmaceutical Discovery/Development)

American Society for Mass Spectrometry (ASMS), June 2022, Minneapolis, MN
Organizer, Workshop: *Machine Learning: How is it enhancing Mass Spectrometry*

American Chemical Society (ACS) National Meeting, Fall 2021, Atlanta, GA
Organizer, *Machine Learning and Automation for Chemistry*
(ACS - ANYL, COMP, CINF Divisions)

American Society for Mass Spectrometry (ASMS), November 2021, Philadelphia, PA
Organizer, Workshop: *Machine Learning: How is it enhancing Mass Spectrometry*

American Society for Mass Spectrometry (ASMS), June 2020, *virtual*
Organizer, Workshop: *Machine Learning: How is it enhancing Mass Spectrometry*

Pittcon, March 2020, Chicago, IL
Organizer, *Machine Learning in Analytical Chemistry* Symposium

American Chemical Society (ACS) National Meeting, Fall 2020, San Francisco, CA
Organizer, *Machine Learning: How is it enhancing Analytical Chemistry?*
(ACS - ANYL Division)

Biophysical Society 62nd Annual Meeting, San Francisco, CA
2018 Co-chair, *Session*: Sensing In Vivo and In Vitro

Critical Assessment for Protein Structure Prediction (CASP)

2008, 2010 Session organizer and chair, *Session*: Junior Scientists Session and Posters

Invited Manuscript Reviewer

Proceedings of National Academy of Sciences; Chemical Science; ACS Central Science; Analytical Chemistry; PLoS Computational Biology; Proteins: Structure, Function and Bioinformatics; Nucleic Acids Research; Bioinformatics; PLoS One; International Journal of Molecular Sciences; ACS Omega; Chemical Engineering Science; Journal of Molecular Biology

Invited Consultant

Consultant, Deciduous Therapeutics Inc., Drug Design, 2019-

Merck & Co, Pharmaceutical Sciences, 2019

Cocrystal Pharma for consulting on polarizable force fields, 2010-2012

Algodign LLC for collaboration on polarizable force fields, 2007

NIH NIGMS Mentoring Workshop for New Faculty in Organic and Biological Chemistry, 2016

Participated in workshop activities including mock reviews and proposal presentations

Interdisciplinary Activities

1. *ACS Central Science Editorial board discussion*

At the 255th ACS National Meeting, I was invited by Editor-in-Chief as a guest of Chris Welch to attend and give my feedback about the future of ACS central science suggesting topics and areas of focus for the journal.

2. Member, PULSe interdisciplinary graduate program (administrative training group: Chemical Biology): interviewed PULSe prospective students: 2016, 2017, 2018

Other affiliations: Molecular Signaling and Cancer Biology, Immunology and Infectious Diseases, Integrative Neuroscience, Computational and Systems Biology

3. Representative from Dept. of Chemistry for Computational Life Science (CLS) program at Purdue (2016-).

4. *Member affiliations*: Purdue Institute for Drug Discovery, Purdue Institute for Integrative Neuroscience, Purdue Institute for Immunology, Inflammation and Infectious Disease, Integrative Data Science Initiative

5. *Full member* - Purdue Center for Cancer Research (Targets, Structures, Drugs). Participated in several events to give talks and engage with companies such as ATOM do to machine learning based drug design to combat cancer. Participation for program project grants is ongoing.

6. *Interdisciplinary Collaborations* – I have established interdisciplinary collaborations withing and outside Purdue that has resulted in funding and publications. These include collaboration with the Colleges of Engineering, Pharmacy and Veterinary Medicine at Purdue University and in the areas of computational modeling, cancer biology and neurology at SUNY Buffalo, Harvard University, New York University, University College – London, etc.

Evidence of Involvement of Students in Research Programs

Graduate students

M.S. and Ph.D. students graduated

1. **Priya Prakash; PhD:** Apr 2021

Thesis Title: Characterizing Microglial Response to Amyloid: From New Tools to New Molecules.

DOI: <https://doi.org/10.25394/PGS.14515074.v1>

Distinctions: PI4D Travel Award (2017), Graduate Women in Science Program (WISP) Travel Grant Award (2018), Purdue Graduate Student Government (PGSG) Travel Grant Award (2018), Alzheimer's Drug Discovery Foundation (ADDF) Young Investigator Fellowship Award (2018), PRF Graduate Research Fellowship (2019-2020), SURF Graduate Student Mentor Award (2019), [Eli Lilly-Stark Research Fellowship in Neurodegeneration \(2020-2021\)](#), [M. G. Mellon Award in Analytical Chemistry \(2021\)](#), [PULSe Outstanding Graduate Student in Research Award \(2021\)](#)

Next Position: Postdoctoral Fellow, NYU Neuroscience Institute (Liddelow Lab)

2. **Jonathan Fine; PhD:** May 2020

Thesis Title: Proton to Proteome: A Multi-scale investigation of Drug Discovery

DOI: <https://doi.org/10.25394/PGS.12269000.v1>

Distinctions: Lynn Fellowship (2015-2016), Purdue Graduate Student Government (PGSG) Travel Grant Award (2018), PCCR Bioinformatics Fellowship (2019), [Merck Rising Star in Analytical Chemistry \(2020\)](#), [Thomas W. Keough Graduate Scholarship Award in Analytical Chemistry \(2020\)](#).

Current Position: Senior Scientist, Merck & Co. Inc.

3. **Sheik Dawood; MS:** May 2020

Current Position: Machine Learning Scientist, Micron Technology

Current graduate and postdoctoral students and other research assistants

Graduate students

Student Name	Entered Program	Start Date (mmm-yy)	Expected Completion (mmm-yy)	Distinctions
Armen Beck	Fall 2017	Oct-17	PhD candidate May-23	
Ahad Hossain	Fall 2017	Oct-17	PhD candidate May-23	Graduate School Summer Research Grant (2019)
Prageeth Wijewardhane	Fall 2017	Oct-17	PhD candidate May-23	Lynn Fellowship

Asarasin Adulnirath	Fall 2018 (PULSe)	May-19	PhD dropped (personal reason)	PRF Graduate Research Fellowship
Matthew Muhoberac	Fall 2019	Oct-19	PhD candidate May-24	Ross Fellowship
Connor Beveridge	Fall 2019	Oct-19	PhD candidate May-24	
Palak Manchanda	Fall 2019	Oct-19	PhD candidate May-24	W. Brooks Fortune Analytical Chemistry Fellow
Harshit Arora	Fall 2019	Oct-19	PhD candidate May-24	Ross Fellowship
Saniya Virani	Fall 2020	Oct-20	PhD May-25	
Sanjay Iyer	Fall 2020	Oct-20	PhD Passed cumes May-25	
Ruilin Yu	Fall 2020	May-21	PhD May-25	
Pooja Saklani	Fall 2020	Jan-22	PhD May-25	
Guang Yang	Fall 2021	Dec-21	PhD May-26	

Research Assistants

Aug 2016-Jun 2019 Wei Zhang (B.S. Computer Science, Purdue University)

Current Position: Graduate Student at University of Southern California

Aug 2018-May 2019 Jerry Hsu (B.S. Computer Science, Envision Center)

May 2016-May 2018 Jordan McGraw (Graduate student, CGT, Envision Center)

Current and previous undergraduate students

Since I joined Purdue in 2016, I have **mentored 32 undergraduate students** from the Departments of Chemistry, Biochemistry, Computer Science, Computer Engineering, Biomedical Engineering, recruited Purdue Undergraduate Research Experience (PURE) international undergraduate students and NSF REU program domestic undergraduate students from across the US. I am extremely proud of 4 undergraduates who have done honors thesis in my group and 2 of them were recipient of the prestigious Dale W. Margerum Undergraduate Research Scholarship. **Undergraduate students in my lab are also co-first authors and co-author in publications.**

Start date Name (year entered in program, department)

Current Undergraduates

Jan 2022- **Victoria Wendt** (College of Health and Human Sciences)
CHM 499; Neuroimmunology

Aug 2019- **Mung Hong Fong** (2019, Chemistry, exchange student)
CHM 499; *Graph based machine learning in Drug Design*

Aug 2019- **Joseph J. Johnston** (2019, Chemistry)
CHM197, CHM 499; *Chemical synthesis for immunomodulation*

Undergraduate Alumni

Purdue students

Jan 2019 – May 2022 **Ryann Davis** (2017, Chemistry)
CHM 499; *Effect of small molecules on cancer cell lines and microglial phagocytosis*
Distinctions: Falker Summer Research Award (2020)

Aug 2021 – May 2022 **Sunita Nhemafuki** (2020, Biomedical Engineering)
CHM 499; *Microglial phagocytosis in chronic inflammation*

Aug 2020 – May 2021 **Lauren Rutherford** (2020, Chemistry)
CHM 197, CHM 499; *Small molecule immunomodulators*

Aug 2020 – Dec 2020 **Haripriya Sakthivel** (2018, Biomedical Engineering)
CHM 499; *Microglial immunomodulation with Amyloid-beta exposure*
(Leave of Absence since Spring 2021)

Jan 2019 – Dec 2020 **Yingqi Chen** (2016, Chemistry, *Honors Thesis*)
CHM 499; *Modular Synthesis of Small Molecule Immunomodulators*
Distinctions: Leighty Scholarship (2019), Undergraduate Stine-Summer Research Award (2019), Summer Undergraduate Cancer Center Research Award (2020).
Current Position: ***Graduate Admission from Purdue University***

Dec 2016 – May 2020 **Elizabeth Thayer** (2016, Chemistry, *Honors Thesis*)
CHM 499; *Characterization of BV2 microglial inflammatory response towards Amyloid-beta*
Distinctions: Emerson Kampen Scholarship (2017), Undergraduate Margerum Summer Research Award (2017), Summer Stay Scholar (2017, 2019), Undergraduate Stine-Summer Research Award (2018), Oblad Scholarship (2018), UIUC Women Chemist Award (2018), Summer Undergraduate Research Fellowship (2019), Leighty Scholarship (2019), [Dale W. Margerum Undergraduate Research Scholarship \(2020\)](#).
Current Position: ***Graduate Student at University of Illinois, Urbana Champagne***

Aug 2016 – May 2020 **Gabrielle C. Williams** (2016, Biochemistry, *Honors Thesis*)
CHM 197, CHM 499; *Small molecules modulating microglial inflammatory response in vitro*
Distinctions: Summer Stay Scholar (2017); Undergraduate Margerum Summer Research Award (2017), Summer Undergraduate Research Fellowship (2018), Purdue Undergraduate Research Symposium award (2018), Purdue Undergraduate Research Symposium Award (2018), Louis Stokes Alliance for Minority Participation (LSAMP) Program award (2019).
Current Position: ***Manufacturing Scientist, Eli Lilly and Company***

Aug 2017- Aug 2019 **Dawn Tilley** (2017, Chemistry)

CHM 197; CHM 499; *Combination drug testing to reduce inflammatory cytokines with microglia*
Distinctions: Undergraduate Falkner- Summer Research Award (2018), Office of Undergraduate Research (OUR) Scholarship (2018-19), Leighty Scholarship (2018-19), Learning beyond the classroom grant (2018).

Current Position: **Cooks Research Inc.**

Jan 2016 – Jun 2019 **Travis C. Lantz** (2015, Chemistry, *Honors Thesis*)

CHM 499; *Analytical methods for rapid purification of recombinant Amyloid-beta*

Distinctions: Undergraduate Falkner- Summer Research Award (2016); Summer Undergraduate Research Fellow (2017); Award at the ECI ACS Undergraduate Research Conference (2017), Undergraduate Stine-Summer Research Award (2018), Virgil St. John Scholarship in Chemistry (2018), Summer Undergraduate Cancer Center Research Award (2018), [Dale W. Margerum Undergraduate Research Scholarship \(2019\)](#), [NSF GRFP Honorable Mention \(2019\)](#).

Current Position: **Graduate Student at Stanford University**

Aug 2018 – May 2019 **Tim Grotzer** (2018, Chemistry)

CHM 197; *Literature review for studying immune suppression in glial cells*

CHM 499; *Experiments on microglia and review of microglia and microbiome interactions*

Jan 2018 – May 2019 **Andrew Wolfram** (2015, Biochemistry)

CHM 499; *Chemical synthesis of immunomodulatory agents*

Current Position: **Graduate Student at Penn State University**

Aug 2018 – Dec 2018 **Yufan Zhang** (2015, Chemistry)

CHM 499; *Chemical synthesis of immunomodulatory agents*

Aug 2016-Dec 2018 **Brandon T. Stewart** (2015, Computer Science)

CHM 499; *StatChem^{LIB}: CPU/GPU library for docking, design and dynamics*

Distinctions: Summer Undergraduate Research Fellow (2017)

Current Position: **Software Engineer at Apple Inc.**

Jan 2018 – Dec 2018 **Jean-Michael Diel**, (2015, Computer Science)

CHM 499; *Deep learning in chemistry*

Current Position: **Graduate Student at Carnegie Mellon University**

Aug 2016-Jun 2018 **Anav Gagneja** (2014, Computer Science)

CHM 499; *Web server for computational drug design*

Distinctions: Outstanding presentation award at the SIAM CSESC conference (2017)

Current Position: **Software Development Engineer at Amazon Inc.**

Jan 2018 – Aug 2018 **Christopher Sculley** (2017, Computer Science)

CHM 499; *Mobile development of the MINT VR chemistry game*

Aug 2017-Dec2017 **Nathaniell Perena** (2017, Chemistry)

CHM 197; *Chemical synthesis of immunomodulatory agents*

Aug 2016-Aug 2017 **Jacob Gifford** (2016, Biochemistry)

CHM 499: *Computational assay for metabolic stability*

Distinctions: Summer Stay Scholar (2017)

Oct 2016-Dec 2016 **Siddharth Inani** (2016, Computer Engineering)
Cando data web application development

Aug 2016-May 2017 **Benjamin M. Collins** (2013, Chemistry)
CHM 499; *Bioanalytical chemistry for Alzheimer disease*
Current Position: ***Territory Sales Manager at Midwest Lab Solutions***

Aug 2016-Jan2017 **Shubhang Kulkarni** (2015, Computer Science)
CHM 499; *Candock code base optimization*

Aug 2016-Jan2017 **Ryan Everett** (2015, Computer Science)
CHM 499; *Multiplayer drug discovery game development*

Aug 2016-May2017 **Wei Zhang**, (2013, Computer Science)
CHM 499; *Multiplayer drug discovery game development*
Current Position: ***Graduate Student at University of Southern California***

Jun 2016-Aug 2016 **Teresa Kennelly** (2015, Chemistry)
Biomarker discovery for Alzheimer's disease
Distinctions: Undergraduate Data Science Award (2016)

Jan 2016-Aug 2016 **Jessup Dowell** (2013, Chemistry)
CHM 499: *Drug repurposing pipelines for orphan diseases*
Distinctions: Undergraduate Stine- Summer Research Award (2016)

NSF REU students

May 2021-Jul 2021 **Crystal Vega** (East Los Angeles College, Chemistry)
NSF-REU Student; *Multifunctional Small Molecule Probes*

May 2021-Jul 2021 **Kevin Yu** (Caltech, Chemistry)
NSF-REU Student; *Generative machine learning for synthetic feasibility*

May 2017-Aug2017 **Brigid Rodrigues**, Junior, University of Dallas, TX

Purdue Undergraduate Research Experience (PURE) students

June 2018-Aug2018 **Anand A Rajasekar**, Indian Institute of Technology (IIT) – Madras, India

June 2018-Aug2018 **Akanksha Yadav**, Indian Institute of Technology (IIT) – Bombay, India

Current and previous postdoctoral associates

Trainee Name	Postdoc Training Period	Prior Academic Degree(s)	Previous Academic Degree Year(s)	Previous Academic Degree Institution(s)	Postdoctoral Research Area	Current Position of Past Trainees
	8/2021—		2018		Microglial Cell Dysfunction	Current

Dr. Kanchan Bisht		PhD, Neurobiology		Laval University, Canada		
Dr. Kaushik Sharma	8/2021—	PhD, Neuroscience	2016	National Brain Research Center, India	<i>In vivo</i> models of chronic neuroinflammation	Current
Dr. Caitlin Randolph <u>Distinction</u> : Arnold and Mabel Beckman Fellowship (2022-24) ; Guy Mellon Award in Analytical Chemistry (2020)	1/2021—	PhD, Chemistry	2020	Purdue University – College of Science	Lipid structural analysis for Immunomodulation of Glial Cells	Current
Dr. Erin Kischuk <u>Distinction</u> : Midwest TME Young Investigator Award (2020)	9/2019— 11/2020	PhD, Immunology	2019	Purdue University – College of Veterinary Medicine	Immunomodulation of Myeloid-derived Suppressors Cells and Microglial Cells	Clinical Scientist, Cook Medical Inc., West Lafayette, IN
Dr. Krupal P. Jethava <u>Distinction</u> Alzheimer's Drug Discovery Foundation Young Investigator	12/2017—	PhD, Chemistry	2017	National Institute of Pharmaceutical Education and Research, India	Small molecule immune modulators and pH sensitive neuronal materials for immune modulation	Current

r Fellowship Award (2019)						
Dr. Joydeb Majumder Distinction s Purdue Postdoc Associatio n Travel Award (2016, 2017)	4/2016— 4/2019	PhD, Chemistry	2016	Indian Association for the Cultivation of Science, Kolkata, India	Cancer drug discovery; Chemical methods for cell surface functionalization	Research Associate, Rutgers University , NJ

Service on MS/PhD committees

Total: 43 students PhD thesis committee member / chair

Graduated shown in red

Chair: 11 PhD students and 1 MS student from my lab

#	Student	Degree	Degree Expected	Participation	Department (Advisor)
1.	Erin Kischuk	Ph. D.	05/2019	Committee Member	Compar. Pathobio. (Ratliff)
2.	Anuradha Bhat	Ph. D.	12/2021	Committee Member	Env. Ecol. Engg. (Harris)
3.	Wanru Li	Ph. D.	05/2022	Committee Member	Chemistry (Kenttämaa)
4.	Moloud Aflaki	Ph. D.	08/2018	Committee Member	Chemistry, PULSe (Sintim)
5.	Yanal Oueis	Ph. D.	05/2021	Committee Member	Chemistry (A. Wasserman)
6.	Shruti Biyani	Ph. D.	05/2022	Committee Member	Chemistry (D. Thompson)
7.	Rong Chen	Ph. D.	05/2022	Committee Member	Chemistry (Cooks)
8.	Bhavani Gopalakrishna	Ph. D.	08/2020	Committee Member	Biomedical Engg. (Solorio)
9.	Elizabeth Larocoue	Ph. D.	05/2020	Committee Member	Chemistry (Sintim)
10.	Yangjie Li	Ph. D.	05/2021	Committee Member	Chemistry (Cooks)
11.	Sunghyun Myoung	Ph. D.	05/2020	Committee Member	Biological Sc. (Kasinski)
12.	Allison Briggs	Ph. D.	05/2020	Committee Member	Biochemistry (Gowher)
13.	Craig Sweet	Ph. D.	08/2019	Committee Member	Chemistry (D. Thompson)
14.	Claudia Viquez-Rojas	Ph. D.	05/2020	Committee Member	Chemistry (Slipchenko)
15.	Jonathan Fine	Ph. D.	05/2020	Committee Chair	Chemistry (Chopra)
16.	Priya Prakash	Ph. D.	05/2021	Committee Chair	Chemistry (Chopra)
17.	Armen Beck	Ph. D.	05/2023	Committee Chair	Chemistry (Chopra)
18.	Ahad Hossain	Ph. D.	05/2022	Committee Chair	Chemistry (Chopra)
19.	Prageeth Wijewarshane	Ph. D.	08/2022	Committee Chair	Chemistry (Chopra)
20.	Asarasin Adulnirath	Ph. D.	05/2022	Committee Chair	Chemistry (Chopra)
21.	Sheik Dawood	M. S.	05/2020	Committee Chair	Elec. Comp. Engg. (Chopra)
22.	Harshit Arora	Ph. D.	05/2024	Committee Chair	Chemistry (Chopra)
23.	Connor Beveridge	Ph. D.	05/2024	Committee Chair	Chemistry (Chopra)

24.	Saloni Darji	Ph. D.	05/2024	Committee Member	Chemistry (D. Thompson)
25.	Rishabh Gupta	Ph. D.	05/2024	Committee Member	Chemistry (S. Kais)
26.	Palak Manchanda	Ph. D.	05/2024	Committee Chair	Chemistry (Chopra)
27.	Yazan Meqbil	Ph. D.	05/2024	Committee Member	MCMP (van Rijn)
28.	Imrul Shahriar	Ph. D.	05/2023	Committee Member	Chemistry (P. Low)
29.	Lan Xu	Ph. D.	05/2019	Committee Member	Chemistry (Kenttämaa)
30.	Matthew Muhoberac	Ph. D.	05/2024	Committee Chair	Chemistry (Chopra)
31.	Dustin Harmon	Ph. D.	05/2024	Committee Member	Chemistry (Simpson)
32.	Aleksandr Razumtcev	Ph. D.	08/2024	Committee Member	Chemistry (Simpson)
33.	Qiyuan Zhao	Ph. D.	05/2023	Committee Member	Chemical Engg. (B. Savoie)
34.	Shahed Haghiri	Ph. D.	08/2025	Committee Member	Chemistry (Slipchenko)
35.	Suraj Ugrani	Ph. D.	12/2022	Committee Member	Chemical Engg. (S. Kim)
36.	Nicolae Iovanac	Ph. D.	08/2021	Committee Member	Chemical Engg. (B. Savoie)
37.	Ruilin Yu	Ph. D.	05/2025	Committee Chair	Chemistry (Chopra)
38.	Saniya Virani	Ph. D.	05/2025	Committee Chair	Chemistry (Chopra)
39.	Sanjay Iyer	Ph. D.	05/2025	Committee Chair	Chemistry (Chopra)
40.	Pooja Saklani	Ph. D.	05/2025	Committee Member	Chemistry (A. Tao)
41.	Lauren B. Blaudeau	Ph. D.	05/2024	Committee Member	Chemistry (Kenttämaa)
42.	Zih-Yu Lin	Ph. D.	05/2023	Committee Member	Chemical Engg. (B. Savoie)
43.	Delmis Hernandez	Ph. D.	05/2022	Committee Member	Chemistry, PULSe (Sintim)

TEACHING ACTIVITIES, ASSIGNMENT & STUDENT EVALUATION

A. Teaching Assignments at Purdue

Semester & Year	Course Number, Credit Hour & Type	Title of Course	# of Students	Student Classification
Spring 2016	CHM 57900, 3 cr, Lecture & Lab	Computational Chemistry (001, 002) – Molecular Modeling & Machine Learning	13	Graduate & Undergraduate (Sr.)
Spring 2016	CHM 69900, 3-18 cr, Research	Research PhD thesis	1	Graduate
Spring 2016	CHM 49900, 1-3 cr, Undergraduate Research	Special Assignment (077)	2	Undergraduate
Summer 2016	CHM 69900, 3-18 cr, Research	Research PhD thesis	1	Graduate
Summer 2016	CHM 49900, 1-3 cr, Undergraduate Research	Special Assignment (038)	1	Undergraduate
Fall 2016	CHM 49900, 1-3 cr, Undergraduate Research	Special Assignment (043, 081)	7	Undergraduate
Fall 2016	CHM 69900, 3-18 cr, Research	Research PhD thesis	2	Graduate
Spring 2017	CHM 57900, 3 cr, Lecture & Lab	Computational Chemistry (001, 002) – Molecular Modeling & Machine Learning	12	Graduate & Undergraduate (Sr.)
Spring 2017	CHM 69900, 3-18 cr, Research	Research PhD thesis	3	Graduate

Spring 2017	CHM 49900, 1-3 cr, Undergraduate Research	Special Assignment (077, 089)	7	Undergraduate
Summer 2017	CHM 69900, 3-18 cr, Research	Research PhD thesis	3	Graduate
Fall 2017	CHM 37300, 3 cr, Lecture	Physical Chemistry	70	Undergraduate
Fall 2017	CHM 69500, 0-1 cr, Lecture	Seminar Physical Chemistry	29	Graduate
Fall 2017	CHM 69900, 3-18 cr, Research	Research PhD thesis	3	Graduate
Fall 2017	CHM 49900, 1-3 cr, Undergraduate Research	Special Assignment (043)	5	Undergraduate
Spring 2018	CHM 57900, 3 cr, Lecture & Lab	Computational Chemistry (001, 002) – Molecular Modeling & Machine Learning	14	Graduate & Undergraduate (Sr.)
Spring 2018	CHM 69500, 0-1 cr, Seminar	Seminar Physical Chemistry (004, 006, 022)	34	Graduate
Spring 2018	CHM 69900, 3-18 cr, Research	Research PhD thesis	6	Graduate
Spring 2018	CHM 49900, 1-3 cr, Undergraduate Research	Special Assignment (077, 092)	7	Undergraduate
Summer 2018	CHM 69900, 3-18 cr, Research	Research PhD thesis	6	Graduate
Fall 2018	CHM 37300, 3 cr, Lecture	Physical Chemistry	82	Undergraduate
Fall 2018	CHM 69500, 0-1 cr, Lecture	Seminar Physical Chemistry	26	Graduate
Fall 2018	CHM 69900, 3-18 cr, Research	Research PhD thesis	5	Graduate
Fall 2018	CHM 49900, 1-3 cr, Undergraduate Research	Special Assignment (043)	7	Undergraduate
Fall 2018	BIOL 695, 2 cr, Seminar	Neurological and Neuropsychiatric Disorders, <i>2 Lectures on Alzheimer's Disease</i> [#]	18	Graduate
Spring 2019	CHM 57900, 3 cr, Lecture & Lab	Computational Chemistry (001, 002) – Molecular Modeling & Machine Learning	6 (Lec) 6 (Lab)	Graduate & Undergraduate (Sr.)
Spring 2019	CHM 69500, 0-1 cr, Lecture	Seminar Physical Chemistry (004, 022)	29	Graduate
Spring 2019	CHM 69900, 3-18 cr, Research	Research PhD thesis	6	Graduate
Spring 2019	CHM 49900, 1-3 cr, Undergraduate Research	Special Assignment (077)	7	Undergraduate
Summer 2019	CHM 69900, 3-18 cr, Research	Research PhD thesis	6	Graduate
Summer 2019	CHM 49900, 1-3 cr, Undergraduate Research	Special Assignment (038)	1	Undergraduate
Fall 2019	CHM 37300, 3 cr,	Physical Chemistry	90	Undergraduate

	Lecture			
Fall 2019	CHM 69500, 0-1 cr, Lecture	Seminar Physical Chemistry (004, 018)	32	Graduate
Fall 2019	CHM 69900, 3-18 cr, Research	Research PhD thesis	7	Graduate
Fall 2019	CHM 49900, 1-3 cr, Undergraduate Research	Special Assignment (043)	4	Undergraduate
Fall 2019	BIOL 695, 2 cr, Seminar	Neurological and Neuropsychiatric Disorders, <i>2 Lectures on Alzheimer's Disease</i> [#]	18	Graduate
Spring 2020	CHM 57900, 3 cr, Lecture & Lab	Computational Chemistry (001, 002) – Molecular Modeling & Machine Learning	16 (Lec) 16 (Lab)	Graduate & Undergraduate (Sr.)
Spring 2020	CHM 69500, 0-1 cr, Lecture	Seminar Physical Chemistry (004, 022)	32	Graduate
Spring 2020	CHM 69900, 3-18 cr, Research	Research PhD thesis	10	Graduate
Spring 2020	CHM 59900, 3 cr, Graduate Research	Special Assignment (007)	1	Undergraduate
Spring 2020	BCHM 49900, 1-3 cr, Undergraduate Research	Honors Thesis in Biochemistry (H26)	1	Undergraduate
Spring 2020	CHM 49900, 1-3 cr, Undergraduate Research	Special Assignment (077)	5	Undergraduate
Summer 2020	CHM 69900, 3-18 cr, Research	Research PhD thesis	9	Graduate
Fall 2020	CHM 37301, 3 cr, Lab	Physical Chemistry Laboratory	84	Undergraduate
Fall 2020	CHM 69500, 0-1 cr, Lecture	Seminar Physical Chemistry (004, 018)	24	Graduate
Fall 2020	CHM 69900, 3-18 cr, Research	Research PhD thesis	9	Graduate
Fall 2020	CHM 49900, 1-3 cr, Undergraduate Research	Special Assignment (043)	3	Undergraduate
Spring 2021	CHM 57900, 3 cr, Lecture & Lab	Computational Chemistry (001, 002) – Molecular Modeling & Machine Learning	12 (Lec) 12 (Lab)	Graduate & Undergraduate (Sr.)
Spring 2021	CHM 69900, 3-18 cr, Research	Research PhD thesis	11	Graduate
Spring 2021	CHM 49900, 1-3 cr, Undergraduate Research	Special Assignment (043)	2	Undergraduate
Fall 2021	CHM 37300, 3 cr, Lecture	Physical Chemistry	80	Undergraduate
Fall 2021	CHM 69900, 9-18 cr, Research	Research PhD thesis	10	Graduate
Fall 2020	CHM 49900, 1-3 cr, Undergraduate Research	Special Assignment (089)	3	Undergraduate
Fall 2021	BIOL 695, 2 cr, Seminar	Neurological and Neuropsychiatric Disorders,	13	Graduate

		2 Lectures on Alzheimer's Disease [#]		
Spring 2022	CHM 57900, 3 cr, Lecture & Lab	Computational Chemistry (001, 002) – Molecular Modeling & Machine Learning	13 (Lec) 13 (Lab)	Graduate & Undergraduate (Sr.)
Spring 2022	CHM 69900, 3-18 cr, Research	Research PhD thesis	12	Graduate
Spring 2022	CHM 49900, 1-3 cr, Undergraduate Research	Special Assignment (043)	5	Undergraduate

This class was organized by PIIN that included faculty lecture and student presentation

B. Course Evaluations -- Student Evaluation

Semester & Year	Course	Response/Enrollment (% response)	C1 Score Median	C2 Score Median
Spr 2021	CHM 579 (Lec, Lab)	9/10 (90%)	4.44*	4.78**
Fall 2020	CHM 37301 (Lab)	84 students	No evaluation was asked for faculty instructors	No evaluation was asked for faculty instructors
Spr 2020	CHM 579 (Lec, Lab)	11/15 (73%)	No evaluation score due to covid-19	No evaluation score due to covid-19
Fall 2019	CHM 373	84/90 (93.33%)	4.1	4.4
Spr 2019	CHM 579 (Lec, Lab)	3/6 (50%)	3.5	3.5
Fall 2018	CHM 373	23/81 (28.40%)	3.9	4.0
Spr 2018	CHM 579 (Lec, Lab)	4/11 (36.36%)	4.2	4.2
Fall 2017	CHM 373	29/70 (41.43%)	3.7	3.8

Spr 2017	CHM 579 (Lec, Lab)	8/12 (66.67%)	4.0	3.9
Spr 2016	CHM 579 (Lec, Lab)	5/12 (41.67%)	3.3	3.7

C1: Overall I will rate this course as (excellent = 5, very poor = 1)

C2: Overall I will rate this instructor as (excellent = 5, very poor = 1)

* The instructor clearly explains material so that I can understand it.

** The instructor seems to care that I learned this material.

ENGAGEMENT ACTIVITIES

A. Department

2021-2022 Analytical Chemistry Faculty Search Committee

Outcome: 1 accepted offer of Associate Professor starting in Summer 2022

Organic Chemistry Adhoc Faculty Search Committee

Outcome: 1 accepted offer of Assistant Professor starting in Fall 2022

2020-2021 Department Representative for College-wide Data Science Faculty Search Committee

Role: Took part in the Physical Science and Biological Science college-wide search.

Regular weekly meetings, review of applications, selection of candidates for interviews, engagement with department head and faculty in multiple divisions in Chemistry to select data science candidates for interviews, conducted interviews, provided feedback and wrote assessment summaries of candidates.

Outcome (Chemistry): 1 accepted offer of Assistant Professor to start in Fall 2021; 1 pending offer after visiting the university in person.

2019-Present Member of the Department Safety Committee

2016-2019 Graduate Admissions and Recruiting Committee,

Domestic & International admissions

Role: All aspects of the admission process from attending meetings, file reviewing, selection and interview of candidates (international), to, attendance in the graduate symposium representing Physical and Analytical divisions.

2016-2017 Member of the Department Facilities and instrumentation committee

B. College

2020- Faculty Council representing Department of Chemistry

2020 College-wide Data Science Faculty Search Committee for Physical and Biological Science

2016 Predictive Science Faculty Cluster Hiring with Engineering, 2016
Role: Meeting with the search candidate and providing feedback

C. University

- 2020- **Engagement with Merck & Co. for funding projects across Purdue University** – Currently projects active in College of Science, College of Engineering, College of Pharmacy – under a *Master Agreement* with projects funded through Purdue Sponsored Program Services.
- 2019 Invited Panelist, Open Data and Publishing, “What does open access mean to you.” Purdue University Libraries and School of Information Studies, 22 October 2019.
- 2018- Reviewer for the Purdue University Center for Cancer Research Pilot Grants
- 2016-2018 *Big data strategic leadership committee in Life Sciences*
Role: Understand capabilities existing in this space on campus, what is needed from a resource and organizational point of view, as well as what we need as a university to be on the leading edge of life sciences moving forward to propose recommendations and roadmaps. Planned a strategic workshop and selection of speakers for Big Data Symposium at Purdue on 20th April 2018.
- 2016-2018 PULSe Graduate Admissions Committee
Role: All aspects of the admission process from attending meetings, file reviewing, selection and interview of candidates visiting Purdue representing Chemical Biology, Cancer, and Computational groups.
- 2017 - *Developing research collaboration with universities/research centers and industries (start-up, etc.) in India* – Engaging with university activities for Undergraduate Research Experience (PURE) student committee and with research partners visiting Purdue University.
- 2016-2018 *Faculty Search committee participation:*
Bindley Director search meetings
Predictive Science faculty cluster hiring search committee, Engineering
Purdue Institute for Integrative Neuroscience Director search
- 2016-2017 MCMP Faculty recruitment participation, College of Pharmacy
Role: Meeting with faculty search candidates on their first or second visits
- 2016 Faculty Search Participation, Department of Biochemistry, Purdue College of Agriculture
Role: Meeting with the search candidate
- 2016- PULSe program, Preliminary examination committees
Role: Served as a Chair of the preliminary exam committee and a member for a total of 10 preliminary examination committees that included reading proposals, providing feedback and attending the oral defense of the proposal by students.

D. Diversity Activities

Diversity is essential for STEM and to engage towards this directly, I have been a co-PI of the NSF REU for past several years that provides research experience to undergraduates. REU is open to all, but student recruitment efforts target underrepresented groups by partnering with 3 universities that have historically served underrepresented students. Undergraduates will complete an independent research project in analytical chemistry mentored by a faculty member and graduate student. To broaden the participation of minority or underrepresented groups in STEM, I am committed to providing research opportunities through the **NSF REU award**, Purdue Undergraduate Research Experience (**PURE**) programs (*visiting students from India*), Summer Undergraduate Research Fellowship (**SURF**), Louis Stokes Alliance for Minority Participation (**LSAMP**) and providing research experience to high school students.

My commitment to diversity, equity, and inclusion. I and my lab has pledged to actively work towards fostering a diverse and inclusive environment for all our members irrespective of their race, color, age, religion, sexual orientation, gender, disability, or national origin. We celebrate and use our differences to better our science. Our goal is to provide our members with a safe space to thrive and pursue their scientific curiosities to their fullest potential.

I am committed towards encouraging women and minority groups to join the scientific workforce. So far, I have mentored 12 female undergraduate students, 4 female graduate and 3 female postdoctoral students, 1 African American undergraduate student, 1 LGBTQ graduate student and 1 LGBTQ undergraduate student. Currently, my lab has 8 female students (1 postdoctoral, 3 graduate and 4 undergraduates) and I strive to keep the ratio of men to women scientists equal to enhance diversity in science. I encourage and support both graduate and undergraduate women in my lab to attend events organized by the *National Honors Society of Women in Chemistry*. Furthermore, I am proud of the fact that currently there are students from 7 different countries who are part of my lab.

High School Students Teaching and Mentorship

Mentored high school students, both before and since arriving to Purdue who have participated and presented in science fair competitions: one student was an undergraduate at Harvard University who was a semifinalist in Intel Science Talent Search and another is a junior in high school who was selected among many for the USA Computing Olympiad and now an undergraduate at MIT.

2018 Teaching sessions using our lab's virtual using reality drug discovery education game (funded by Purdue Instructional Innovation Award) to high school teachers and students from all over Indiana for a Chemistry AP student event organized by Sarah Nern.

2018- **Rithvik Ganesh** (Jasper High School, Plano, TX)
Combination drug toxicity and prescription recommendations using protein-drug interactome signatures

2016-2018 **Aayush Gupta** (Sophomore, Saratoga High School, CA)
Combination drug toxicity and prescription recommendations using protein-drug interactome signatures
Current position: Undergraduate in Computer Science, MIT.

2012-2014 **Vikram Sundar** (The Harker School, San Jose, CA, before Purdue)
Incorporating flexibility in protein-protein docking.
Current position: Artificial Intelligence Resident, Google.

E. Other Engagement Activities and Outreach

We have also initiated additional industry collaborations who are interested in using the technologies coming out of my lab in collaboration or as part of their service. We have signed CDA with PRF and have engaged talks at different levels with these potential industry partners.

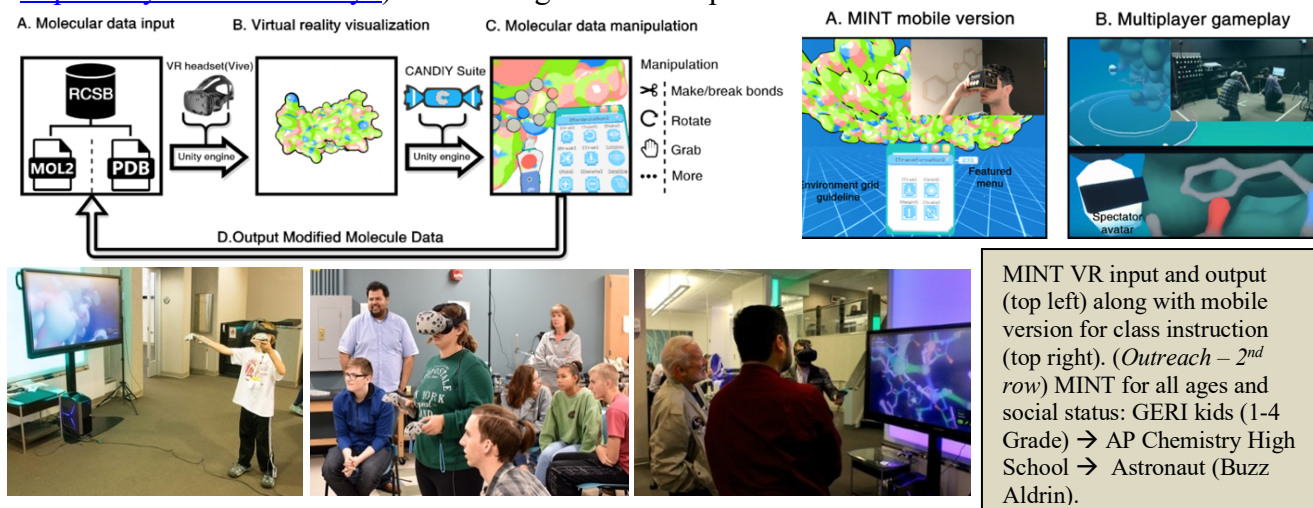
1) Industry / Sponsor collaborations and signed CDA with Purdue PRF

- Indiana Biosciences Research Institute – Drug design for Diabetes (type 1 and 2)
- Deciduous Therapeutics Inc. – Small molecule drug design
- Moron Bioventures – Interested in our patented cell-conjugation technology
- Systems Oncology – Machine learning method to design and synthesize immunomodulators
- Mercury Fund – Data-based drug discovery and immunomodulation
- Cyclica, Inc. – Interactome based drug design technology
- INmune Bio. – Cell-drug conjugation methods we are developing for immune cells
- Allvirez, Inc. – SBIR/STTR - Design and synthesis of compounds to combat HIV
- Merck & Co.. – Funding for peptide aggregation modeling
- OnAI Inc. – NSF SBIR Funding for covid-19 distributed blockchain implementation

2) Virtual reality based multiplayer drug discovery game for education and science

Game frontend development in collaboration with Purdue Envision Center based on our drug design methods

Summary: We have developed a virtual reality (VR) chemistry software for medicinal chemistry and structural biology powered by the chemical docking and design software from my lab. We call this VR software MINT (Molecular Interactions using New Technologies) which is a virtual reality based “drug discovery game.” MINT was funded by the *Instructional Innovation Award* and we specified its development and algorithms in the manuscript for molecular visualization, manipulation and instruction (**chemRxiv** 9889994 [Preprint]. doi: <https://doi.org/10.26434/chemrxiv.9889994.v1>). MINT is used for our research and outreach efforts for education and science. We have done several educational outreach events (shown below). In future, we plan to give out important drug targets that are active areas of research in my lab to the community and the best scored prediction from any “citizen scientist” will be tested experimentally. If the results are validated and we write papers based on his/her prediction, the person who identified the best result will be a co-author on the paper. We have already released v1.0 of our MINT software publicly to download from the Chopra group webpage. We believe this is a good approach for MINT to be discovered in different parts of the world, and we expect it will be played by chemists and lay public alike (Figure). We have already made VR Google Cardboard ready tutorials freely available on our YouTube Channel ([chopralab - https://tinyurl.com/z5tachy9](https://tinyurl.com/z5tachy9)) showcasing basic concepts of intermolecular forces that can be viewed



with any smart phone on our channel. We have also developed several **interactive tutorials** for mobile devices to give a VR experience independently and these have been used in conjunction with the desktop VR headset in a multiplayer manner as part of student-teacher instruction (Figure). A version of **MINT Mobile app** on Google Play Store for Android already exists for download (https://play.google.com/store/apps/details?id=com.Chopralab.Mint&hl=en_US&gl=US).

Outreach: Science Express has already deployed the game in Science Express vans to go all over Indiana's schools K-12. I was involved in a teaching session about this technology with high school teachers from all over Indiana for an event organized by Sarah Nern. The educational portion of the game will be implemented in Chemistry graduate and undergraduate courses to teach molecular interactions..

C&EN News coverage for MINT VR demo at the 255th ACS Annual Meeting in New Orleans: <https://www.facebook.com/CENews/videos/10160015063650265/> ; **Other media** – https://www.itap.purdue.edu/newsroom/news/170421_DrugDiscoveryGame.html <https://www.science.purdue.edu/e-newsletters/fall2016/Chopra-VR-game.html> https://www.itap.purdue.edu/newsroom/news/170303_EnvisionCenter_PresidentDaniels.html <https://www.rcac.purdue.edu/news/961>

Education Outreach

I am passionate about outreach and engagements with communities, schools and colleges, specifically related to enhancing impact for underrepresented minorities in STEM. We made extensive efforts towards partnering with several schools and communities of children to enhance their love for science. Since 2017, in collaboration with the Envision Center at Purdue and the Purdue Science Express, our MINT VR education gaming platform has been used for several outreach events, summer camps and tours *covering attendees from K-12 all the way to retirement communities* to enhance their love for chemistry and learning as a fun interactive game that is suitable for all ages (Figure). Purdue Science Express vans go all over Indiana schools to showcase our MINT VR gaming platform to spark an interest in science. Since there is no age limit to play MINT, we also get encouragement from younger K-12 students and have included this as part of several younger students outreach efforts.

- Purdue Day at the Statehouse – Science Express Event Invitation for MINT Demo for STEM, research
 - 02/18/2019
- Molecular Modeling lab using MINT VR chemistry game for AP Chemistry High School students
 - 10/12/2018
- TEAM: Technology Expanding All Minds - 8-10th grade students for women in technology
 - 6/27/2017
- TAGS: Technology Advancing Girl Scouts 6-8th grade Girl Scouts of Indiana to Purdue Polytechnic
 - 7/19/2017
- TOTAL: Turned onto technology and leadership: 7-9th grade students towards technology, innovation, teamwork and creative thinking
 - 6/14/2017
- Deaf Kids Code: Promotes technology/computing skills as an innovative tool to empower deaf/hard of hearing students socially and economically
 - 4/2/2017
- College Mentors for Kids: Big buddies program at college to mentor children to improve lives through encouraging education.

- 4/6/2017
- Westminster Village: Retirement community in West Lafayette. We ran a tour to highlight Purdue research and education programs.
 - 7/18/2017
- GERI program: students from Grades 1-4
 - 6/14/2017
- Gifted high school biochemistry summer camp (Organizers: Stefan Paula and Mark Hall)
 - 7/10/2017: Students experienced the VR visualization and binding site of the drug target
- Dawn or Doom 2017:
 - 9/26-27/2017

3) Software and web server development

Full software repositories publicly available at <https://github.com/chopralab>

- **Glial Cells Proteomics, Lipidomics and Metabolomics Portal:** Web application for microglia and astrocytes cells omics resource for the data generated in our laboratory on these cells.
<http://gliaomics.com>
<http://microgliaomics-chopralab.appspot.com> (login: admin ; password: Review)
- **CANDIY (Chemical Algorithms for Network based Decisions on Interactions for modeling reactivity)**
<https://github.com/chopralab/candiy>
- **LEMON:** Data mining and feature generation framework for machine learning on structural data. Usermanual available at – <https://chopralab.github.io/lemon/latest/>
- **Machine Learning for Chemistry Reactivity**
 Interpretable Machine learning for Chemical Reactions. N-sulfonylimines Reaction Mechanism website: https://chopralab.github.io/n_sulfonylimine_reactions/
 Code: https://github.com/chopralab/n_sulfonylimine_reactions
- **Graph based machine learning for Drug Design.** Energy based graph neural network software:
<https://github.com/chopralab/egnn>
- **Machine Learning for Analytical Chemistry**
 Neural Networks for Spectroscopy: https://github.com/chopralab/candiy_spectrum
 Interpretable Machine Learning for diagnostic ion-molecule mass spectrometry reactions:
https://github.com/chopralab/mop_reactivity_analysis
- **PADDY – A Genetic Optimization Algorithm for Chemical System and Spaces.**
 User manual: <https://chopralab.github.io/paddy/>
 GitHub code: <https://github.com/chopralab/paddy>
- **SPEAR – Statistical Platform for Elucidating Molecular Reactivity.** Use in molecular simulations to identify transition states on the fly. Code: <https://github.com/chopralab/spear>
- **KoBaMIN – Knowledge Based MINimization server for protein structure refinement**
<http://chopra-modules.science.purdue.edu/modules/kobamin/html/>

Knowledge based minimization server for protein structure refinement with stereochemistry optimization and calculation of C α RMS, GDT-TS and GDT-HA with the reference structure.

- **BINDNET** - Predict BINDing NETwork between proteomes and small molecules
<http://protinfo.org/cando/modules/bindnet>
Predict interaction of between user specified small molecules with selected structural proteomes of interest.
- **CANDOCK** – Fast and flexible protein information based ligand docking
<http://protinfo.org/candock/candock-server>
A flexible protein-ligand docking methodology to predict structures of protein/ligand complexes. Given a protein structure, a ligand, and a binding site location, this module will determine five different possible protein/ligand poses. For each pose, the module reports a score that assesses the goodness-of-fit, or likelihood, that the given pose is a physically realistic. If no binding site is given the server will predict the location of functionally relevant binding site.
- **BITS** - Binding site Information To guide model Selection
<http://protinfo.org/cando/casp/bits/>
A computational protocol for model quality assessment using binding site comparisons to judge the quality of the models using the premise that binding sites are more conserved than sequence or structure.
- **STRINGS** - Selection of Templates Recursively by INteGrating exhaustive Strategies
<http://protinfo.org/cando/casp/strings>
Automated protein 3D structure prediction server. Split the protein sequence recursively, align different combinations to identify domains and use multiple templates for modeling. Final selection based on threading and alignment scores.
- **MATRIX** - Methodology for Accurate Template Recognition for predictIng X [=proteins]
<http://protinfo.org/cando/casp/matrix>
Automated protein 3D structure prediction server. Multiple threading programs and templates used for alignment. Combine restraints from multiple threading alignments and select templates by combining binding site information.