Kushol Gupta, Ph.D.
Curriculum Vitae

Date: November 13th, 2024

Address: 901C Stellar-Chance Building | 422 Curie Blvd.
Department of Biochemistry and Biophysics
Perelman School of Medicine, University of Pennsylvania
Philadelphia, P.A. 19104

U.S. Citizen

Education:

2003	Ph.D.	Perelman School of Medicine, University of Pennsylvania (Pharmacology)
1997	B.A.	University of Pennsylvania (Biochemistry and Music)

Postgraduate Training and Appointments:

2023 - Present	Member, Institute for RNA Biology, Perelman School of Medicine, University of Pennsylvania
2023 - Present	Member, Institute for Structural Biology, Perelman School of Medicine, University of Pennsylvania
2017 - Present	Member, Graduate Group in Biochemistry and Biophysics, Perelman School of Medicine, University of Pennsylvania
2017 - Present	Faculty Director, Johnson Foundation Structural Biology and Biophysics Core, Perelman School of Medicine, University of Pennsylvania
2016 - Present	Member, Center for AIDs Research (CFAR), University of Pennsylvania
2016 - Present	Research Assistant Professor, Perelman School of Medicine, University of Pennsylvania, Department of Biochemistry and Biophysics
2010 - 2015	Research Associate, Perelman School of Medicine, University of Pennsylvania, Department of Biochemistry and Biophysics, Laboratory of Gregory Van Duyne, Ph.D.
2008 - 2010	amFAR Mathilde Krim Fellow in Basic Biomedical Research
2007 - 2008	Visiting HHMI Postdoctoral Teaching Fellow**,** Swarthmore College Department of Chemistry and Biochemistry, Swarthmore, P.A.
2003 - 2010	Postdoctoral Fellow, Perelman School of Medicine, University of Pennsylvania & Howard Hughes Medical Institute, Department of Biochemistry and Biophysics, Laboratory of Gregory Van Duyne, Ph.D.

Other Appointments:

2005 Adjunct Lecturer, University of the Arts, Philadelphia, PA.

Awards, Honors and Membership in Honorary Societies:

2008 Rigaku Corporation Postdoctoral Travel Bursary Award

2002 Solomon Erulkar Traveling Fellowship (Intramural) – "DOCK Studies of the PGHS-1 Peroxidase Active Site." Laboratory of Irwin Kuntz (UCSF)

2001 American Heart Association Predoctoral Fellowship, Pennsylvania-Delaware Affiliate.

1997 Nassau Fund Award for Undergraduate Research (Intramural)

Memberships in Professional and Scientific Societies and Other Professional Activities:

2023 Reviewer, Center for Undergraduate Research and Fellowships, University of Pennsylvania (Intramural)

2023 Bioscience Panelist, Neutrons for the Future Workshop, NIST Center for Neutron Research

2022 – Present Member, Cornell CHESS User Executive Committee (UEC) (Deputy Chair, 2023, Chair, 2024 – Present)

2022 Advisor, Road2Research (Penn)

2022 Panelist, NSLSII Structural Biology Workbench, February 3rd, 2022 (Virtual)

2022 – Present Reviewer, NSLS-II Structural Biology Proposal Review Panel

2022 – Present Representative for ACA, American Institute of Physics (AIP) Federation of Societies

2021 – Present Instrument Advisory Committee, CENTAUR-STS (Oak Ridge National Labs)

2021 – Present Secretary, American Crystallographic Association

2021 Featured Subject, "*The Instrumental Chemist*" (A documentary on Arnold O. Beckman)

2020 – Present Skype a Scientist Program Volunteer Speaker

2020 NSF SBIR Study Section

2019 – Present APS BioCAT External Advisory Committee (Chair, 2023-Present)

2019 – Present Proposal Reviewer, Stanford Synchrotron Research Laboratory (SSRL)

2019 – Present Member, Northwest Biophysics Consortium

2019 – Present	Principal Investigator, Beamtime Allocation Cohort (BAG) comprised of investigators from Penn, CHOP, FCCC, and Wistar for X-ray Crystallography, X-ray Footprinting, and Small-Angle Scattering use at NSLSII/BNL.
2018	Chair, Small Angle Neutron Scattering, NSF Prospects in Neutron Scattering for the Biological Sciences Committee Meeting
2018	Grant Reviewer, BBSRC
2017	Chair, Small Angle Scattering Special Interest Group, American Crystallographic Association
2017 – 2018	Reviewer for Center for Nanomaterials (NSLSII)
2016	Chair-Elect, Small Angle Scattering Special Interest Group, American Crystallographic Association
2014 – Present	Proposal Reviewer, CHESS, Cornell University (SAXS)
2012 – Present	Member, Beam Time Allocation Committee, NIST Center for Neutron Research, Gaithersburg, Maryland (SANS)
2011	Contributing Illustrator, "*HIV: From Biology to Prevention and Treatment*" by Frederic D. Bushman, Gary J. Nabel, and Ronald Swanstrom. Cold Spring Harbor Laboratory Press, 2011.
2010 – Present	Proposal Reviewer, Oak Ridge National Laboratory (SANS)
2003 – Present	American Crystallographic Association
2003 – Present	Penn Annual Proseminar Series for New Student Orientation

<u>Editorial Positions (Ad-Hoc):</u>

2024	Reviewer for Archives of Biochemistry and Biophysics
2023	Reviewer for Communication Biology
2023	Guest Editor, Acta. Cryst F, Special Issue on "*Sample Preparation for Structural Biology*"
2022	Reviewer for Current Opinion in Chemical Biology
2022	Reviewer for Protein Science
2022	Reviewer for Viruses
2021	Reviewer for Child Maltreatment

2020	Reviewer for Biochemistry
2019	Reviewer for Methods
2019	Reviewer for FEBS Journal
2019	Reviewer for Biophysical Journal
2018	Reviewer for Biochemical Journal
2018	Reviewer for Nature Communications
2017	Reviewer for Acta Crystallographica-Section F
2017	Reviewer for JoVE
2016	Reviewer for Scientific Reports
2016	Reviewer for Journal of Molecular Graphics and Modelling
2015	Reviewer for Structure
2014	Reviewer for Acta Crystallographic-Section C
2014	Reviewer for The European Biophysics Journal
2014	Reviewer for The Journal of Biological Chemistry
2013	Reviewer for Nature Methods

Academic and Institutional Committees:

1998 - 2001	Student Representative, Admissions Committee, Department of Pharmacology, Perelman School of Medicine, University of Pennsylvania
2017 – Present	Member, Departmental Core Committee, Department of Biochemistry and Biophysics, Perelman School of Medicine, University of Pennsylvania
2022 – Present	Member, Diversity, Inclusion, and Equity Committee, Department of Biochemistry and Biophysics, Perelman School of Medicine, University of Pennsylvania
2024 – Present	Member, Admissions Committee, Department of Biochemistry and Biophysics, Perelman School of Medicine, University of Pennsylvania

Major Academic and Clinical Teaching Responsibilities:

2020 – 2023	Drexel University College of Medicine, BIOC 520S: Macromolecular Structure and Function Course, lecture on Small-Angle Scattering
2019 – Present	Perelman School of Medicine, BMB 555: Macromolecular Crystallography, lectures in X-ray diffraction
2017 – Present	Perelman School of Medicine, BMB 509: Structural and Mechanistic Biochemistry, lecture in Biophysical Instrumentation
2012 – Present	Perelman School of Medicine, BMB 508: Macromolecular Biophysics - Principals and Methods, lectures in Scattering and X-ray Diffraction
2007 – 2008	Swarthmore College Department of Chemistry and Biochemistry. Full-semester undergraduate courses: Chemistry 108: Topics in Biochemistry (Seminar) and Chemistry 45C: Biophysical Chemistry (Laboratory and Lecture)
2005	University of the Arts, Philadelphia, P.A., Full-semester undergraduate course: HU389: Evolution in Modern Perspective
2003	Perelman School of Medicine, PHRM 600: Medical Pharmacology. Lectures in Immunology and Microbiology

Lectures by Invitation:

December, 2024	Workshop Instructor, Everything BioSAXS 10, Advanced Photon Source, Argonne, Illinois.
July, 2024	"Insights into mRNA lipid nanoparticle polydispersity and shape using quantitative solution biophysics" 2024 American Crystallographic Association Meeting, Denver, Colorado.
June, 2024	"Insights into mRNA lipid nanoparticle polydispersity and shape using quantitative solution biophysics" Waters/Wyatt Technologies Webinar.
April, 2024	"Biophysical Studies of mRNA LNPs" Mid-Atlantic Vaccine & Gene Therapy Workshop, Wyatt Technology. New Castle, D.E.
January, 2024	"Emerging Methods in the Biophysical Characterization of mRNA LNPs." New England Structural Biology Association (NESBA) Workshop on SAXS, Vertex Pharmaceuticals, Boston, Massachusetts.
December, 2023	"Structural Intermediates of Phenylalanine Hydroxylase Revealed by Disruption of a Key Intramolecular Interaction." Perelman School of Medicine, University of Pennsylvania, Department of Biochemistry & Biophysics Annual Retreat, Skytop, Pennsylvania.

July, 2023 "Long-Range Structural Effects of ALLINI Resistance Mutations on the Formation of Drug-induced Branched Polymers of HIV-1 Integrase." The 7th International Conference on Retroviral Integration, Boulder, Colorado.

July, 2023 "Structural Intermediates of Phenylalanine Hydroxylase Revealed by Disruption of a Key Intramolecular Interaction." 2023 American Crystallographic Association Meeting, Baltimore, Maryland.

April, 2023 "Structure of a Minimal HIV-1 IN-Allosteric Inhibitor Complex at 2.93 Å Resolutions: Routes to Inhibitor Optimization." National Institutes of Health, Bethesda, Maryland.

February, 2023 Workshop Instructor, Small Angle Scattering Workshop. Advanced Photon Source, Argonne, Illinois. **virtual*

September, 2022 Workshop Instructor, Structural Biology Workbench, National Synchrotron Light Source II, Upton, New York. **virtual*

July, 2022 "Structure of a Minimal HIV-1 IN-Allosteric Inhibitor Complex at 2.93 Å Resolutions: Routes to Inhibitor Optimization." 2022 American Crystallographic Association Meeting, Portland, Oregon.

May, 2022 "Structure of a Minimal HIV-1 IN-Allosteric Inhibitor Complex at 2.93 Å Resolutions: Routes to Inhibitor Optimization." 2022 Retrovirus Meeting, Cold Spring Harbor, New York.

July, 2021 "Solution Conformations of Dimeric Phenylalanine Hydroxylase." 36th Annual Protein Society Meeting. **virtual-COVID-19*

June, 2021 "Assembly of higher-order SMN oligomers is essential for metazoan viability and requires an exposed structural motif present in the YG zipper dimer." 2021 CureSMA Meeting. **virtual COVID-19*

February, 2021 "Studying Macromolecules in Mixtures using Mechanical Marvels" Beckman-Coulter Corporation Webinar

November, 2020 "Allosteric Inhibition of HIV Integrase: Augmenting Crystallographic Studies with Solution Scattering Methods" National Synchrotron Light Source II, Upton, N.Y. **virtual-COVID-19*

October, 2020 Workshop Instructor, Small Angle Scattering Workshop. Advanced Photon Source, Argonne, I.L. **virtual-COVID-19*

March, 2020 "Structural Basis for Inhibitor-Induced Aggregation of HIV Integrase" Rowan College, Department of Chemistry and Biochemistry, Glassboro, N.J.**cancelled – COVID 19*

December, 2019 "Structural Basis for Inhibitor-Induced Aggregation of HIV Integrase" Drexel University College of Medicine, Department of Biochemistry and Molecular Biology, Philadelphia, P.A.

November, 2019 Workshop Instructor, Small Angle Scattering Workshop. Advanced Photon Source, Argonne, I.L.

July, 2019 "Hierarchical structures of HIV Integrase: Drug-induced Aggregates of HIV Integrase are Weak Gels" 2019 American Crystallographic Association Meeting, Cincinnati, O.H.

July, 2018 "Hierarchical structures of HIV Integrase: Drug-induced Aggregates of HIV Integrase are Weak Gels" 2018 American Crystallographic Association Meeting, Toronto, Canada.

April, 2018 Workshop Instructor, "BioSAXS Essentials: Getting Started in Biological Small-Angle X-ray Solution Scattering." CHESS, Cornell University, N.Y.

April, 2018 "Structural Basis for Inhibitor-Induced Aggregation of HIV Integrase" Dickinson College, Department of Chemistry, Carlisle, P.A.

February, 2018 "Applications of Light Scattering to HIV Integrase Structural Biology and Drug Discovery, "Wyatt Technology Corporation Webinar

June, 2017 "Structural Basis for Inhibitor-Induced Aggregation of HIV Integrase" 2017 CHESS User's Meeting, Ithaca, N.Y.

May, 2017 Workshop Instructor, "BioSAXS Essentials: Getting Started in Biological Small-Angle X-ray Solution Scattering." CHESS, Cornell University, N.Y.

May, 2017 "Structural Basis for Inhibitor-Induced Aggregation of HIV Integrase" 2017 American Crystallographic Association Meeting BioSAXS Workshop, New Orleans, L.A.

April, 2017 "Biophysical Studies of Drug Targets" Mid-Atlantic Protein & Biotech Regional User Meeting, Wyatt Technology. Princeton, N.J.

July, 2016 "Applications of Scattering to Structural Biology" 2016 American Crystallographic Association Meeting BioSAXS Workshop, Denver, C.O.

June, 2016 "Structural Basis for Inhibitor-Induced Aggregation of HIV Integrase" 2016 NIH HIV/AIDS Structural Biology Meeting, Bethesda, M.D.

May, 2016 Workshop Instructor, "BioSAXS Essentials: Getting Started in Biological Small-Angle X-ray Solution Scattering." CHESS, Cornell University, N.Y.

July, 2015 "Sample Preparation for BioSAXS, "2015 American Crystallographic Association Meeting BioSAXS Workshop, Philadelphia, P.A.

April, 2015 "Lasers and X-rays and Neutrons (Oh My!) – Applications of Scattering to Structural Biology" Mid-Atlantic Protein & Biotech Regional User Meeting, Wyatt Technology. Princeton, N.J.

October, 2014 Workshop Instructor, "BioSAXS Essentials: Getting Started in Biological Small-Angle X-ray Solution Scattering." CHESS, Cornell University, N.Y.

February, 2014 "Dilemmas, Obstacles, and Challenges in the Structural Study of Large Nucleoprotein Assemblies: The Nucleosome" Collaborative Computational Project for Advanced Analyses Structural Data in Chemical Biology and Soft Condensed Matter (CCP-SAS) Kickoff Meeting, NIST Center for Neutron Research, Gaithersburg, M.D.

July, 2013 "SAXS/SANS Combined with X-ray Crystallography and Computation: Application of Ensemble Analysis Using SASSIE" 2013 American Crystallographic Association Meeting BioSAXS Workshop, Honolulu, H.I.

July, 2013 "The Tyranny of the Lattice: Small-Angle Scattering Studies of Large Nucleoprotein Assemblies." GlaxoSmithKline, Collegeville, P.A.

March, 2013 Workshop Instructor, "BioSAXS Essentials: Getting Started in Biological Small-Angle X-ray Solution Scattering." CHESS, Cornell University, N.Y.

February, 2012 Workshop Instructor, "BioSAXS Essentials: Getting Started in Biological Small-Angle X-ray Solution Scattering." CHESS, Cornell University, N.Y.

November, 2011 "The Tyranny of the Lattice: Small-Angle Scattering Studies of Retroviral Integrases." Stockton College, Department of Chemistry, Galloway, N.J.

October, 2011 The Tyranny of the Lattice: Small-Angle Scattering Studies of Retroviral Integrases." National Synchrotron Light Source, Upton, N.Y.

July, 2011 Workshop Instructor, Summer School on Modeling Neutron Data of Biological Systems. NIST Center for Neutron Research, Gaithersburg, M.D.

June, 2011 "The Tyranny of the Lattice: Small-Angle Scattering Studies of Retroviral Integrases." Department of Biochemistry, Drexel College of Medicine, Philadelphia, P.A.

May, 2011 Workshop Instructor, "BioSAXS Essentials: Getting Started in Biological Small-Angle X-ray Solution Scattering." CHESS, Cornell University, N.Y.

March, 2011 Workshop Instructor, "BioSAXS Essentials: Getting Started in Biological Small-Angle X-ray Solution Scattering." CHESS, Cornell University, N.Y.

October, 2008 "Small-Angle Scattering Studies of HIV IN-LEDGF-DNA Complexes." Department of Biochemistry, Drexel College of Medicine, Philadelphia, P.A.

Organizing Roles in Scientific Meetings:

2025 Co-organizer, "An Introduction to Complementary Solution Biophysics for the Structural Biologist" American Crystallographic Association Meeting, Lombard, I.L.

2024 Co-organizer, "Applications of Small Angle Scattering to Structural Biology: An Introduction" American Crystallographic Association Meeting, Denver, C.O.

2024 Co-chair, “Biotherapeutics and Drug Development: SAXS/SANS/Hybrid Methods.” American Crystallographic Association Meeting, Denver, Colorado.

2024 Organizer, “Minisymposium: Modern Applications of Analytical Ultracentrifugation.” University of Pennsylvania, Philadelphia, P.A. February 20th, 2024.

2023 Co-organizer, “SAMPREP (Sample Attributes for Multiple Techniques and Principal Requirements for Experiments in Pan-structural Biology) Workshop.” American Crystallographic Association Meeting, Baltimore, Maryland.

2023 Co-organizer, “Structural Mass Spectrometry Symposium, in honor of Walter Englander, Ph.D.,” University of Pennsylvania, Philadelphia P.A., May 16th, 2023.

2022 Organizer, “Minisymposium: Modern Applications of Analytical Ultracentrifugation.” University of Pennsylvania, Philadelphia, P.A. October 18th, 2022.

2022 Co-organizer, “Applications of Small Angle Scattering to Structural Biology: An Introduction” American Crystallographic Association Meeting, Portland, Oregon.

2021 Chair, Biological Materials, “New Science Opportunities with Small and Wide-Angle Neutron Diffractometer/Spectrometer at Second Target Station” Oak Ridge National Laboratory. **virtual-COVID-19*

2021 Co-organizer, “Membrane protein structure in membrane and membrane-mimetic environments” American Crystallographic Association Meeting, Baltimore, M.D. **virtual-COVID-19.*

2020 Co-organizer, “Applications of Small Angle Scattering to Structural Biology: An Introduction” American Crystallographic Association Meeting, San Diego, C.A.**virtual – COVID-19*

2019 Organizer, “Minisymposium: Modern Applications of Analytical Ultracentrifugation.” University of Pennsylvania, Philadelphia, P.A. October 15th, 2019.

2019 Co-chair, “SAS Contrast Methods in Biology and Soft Matter” American Crystallographic Association Meeting, Cincinnati, O.H.

2018 Co-organizer, “Applications of Small Angle Scattering to Structural Biology: An Introduction” American Crystallographic Association Meeting, Toronto, Canada.

2017 Organizer, “Minisymposium: Modern Applications of Analytical Ultracentrifugation.” University of Pennsylvania, Philadelphia, P.A. October 18th, 2017.

2017 Session Co-chair, “Integrative Approaches to Structural Biology” 2017 American Crystallographic Association Meeting, New Orleans, L.A.

2016 Organizer, “Minisymposium: Modern Applications of Analytical Ultracentrifugation.” University of Pennsylvania, Philadelphia, P.A. October 18th, 2016.

2016 Session Co-chair, "SAS and Integrative Approaches to Complex Structures." 2016 American Crystallographic Association Meeting, Denver, C.O.

2016 Co-organizer, "Computational Approaches to the Structural Modelling of Biological Macromolecules using Small-Angle Scattering." American Crystallographic Association Meeting, Denver, C.O.

2015 Session Co-chair, "Application of SANS/SAXS to Structural Biology." 2015 American Crystallographic Association Meeting, Philadelphia, P.A.

2015 Organizing Committee, "Small-angle Scattering: Structural Biology and Soft Matter." American Crystallographic Association Meeting, Philadelphia, P.A.

2014 American Conference on Neutron Scattering (ACNS) Program Committee - Biology. Washington, D.C.

Research Publications, peer-reviewed (print or other media):

1. Lee HO, Wang L, **Gupta K**, Dunbrack RL, Majtan T, Kruger WD. Impact of primary sequence changes on the self-association properties of mammalian cystathionine beta-synthase enzymes. *Accepted*, Protein Science (2024).

2. Cory MB, Li A, Hurley CM, Carman P, Pumroy RA, Hostetler ZM, Venkatesh Y, **Gupta K**, Petersson EJ, Kohli RM. The LexA-RecA* structure reveals a lock-and-key mechanism for SOS activation. *Accepted*, Nature Structural and Molecular Biology (2024).

3. Eilers G*, **Gupta K***, Allen A, Montermoso S, Murali H, Sharp R, Hwang Y, Bushman FD, Van Duyne G. Structure of a HIV-1 IN-Allosteric inhibitor complex at 2.93 Å resolution: Routes to inhibitor optimization. PLoS Pathog. 2023 Mar;19(3):e1011097. doi: 10.1371/journal.ppat.1011097. (*=co-first authors)

4. Faylo JL, van Eeuwen T, **Gupta K**, Murakami K, Christianson D. Order in the Core: Transient Prenyltransferase-Cyclase Association in Bifunctional Fuscoccadiene Synthase. Biochemistry 61(21):2417-2430 (2022).

5. Cupo RR, Rizo AN, Braun GA, Tse E, Chuang E, **Gupta K**, Southworth DR, Shorter J. Unique structural features govern the activity of a human mitochondrial AAA+ disaggregase, Skd3. Cell Reports 40(13):111408 (2022).

6. Doll SG, Meshkin H, Bryer AJ, Li F, Ko YH, Lokareddy RK, Gillian R, **Gupta K**, Perilla JR, Cingolani C. Recognition and phosphorylation of the TDP-43 Nuclear Localization Signal. Cell Reports 39(13):111007 (2022).

7. Xia P, Dutta A, Koppula A, **Gupta K**, Batish M, Parashar V. Structural basis of oligoadenylate binding by Csa3 transcription factors. Journal of Biological Chemistry 298(2):101591 (2021).

8. **Gupta K**, Wen Y, Ninan NS, Raimer AC, Sharp R, Spring AM, Johnson MC, Van Duyne GD, Matera AG. Assembly of higher-order SMN oligomers is essential for metazoan viability and requires an exposed structural motif present in the YG zipper dimer. Nucleic Acids Research 49(13):7644-7664 (2021).

9. **Gupta K**, Allen A, Giraldo C, Eilers G, Sharp R, Hwang Y, Cruz K, Janmey P, Bushman F, Van Duyne GD. Drug-induced aggregates of HIV-1 Integrase are branched polymers with the properties of weak gels. Structure 29(3):213-225 (2021).

10. Arturo EC, Merkel G, Hansen MR, Lisowski S, R, Almeida D, **Gupta K**, Jaffe EK. Manipulation of a cation-π sandwich expands knowledge of the conformational flexibility of mammalian phenylalanine hydroxylase. Biochimie 183:63-77 (2020).

11. Eilers, G, **Gupta K**, Allen A, Zhou J, Hwang Y, Cory MB, Bushman FD, Van Duyne G. Influence of the amino-terminal sequence on the structure and function of HIV integrase. Retrovirology 17(1): 28, (2020)

12. **Gupta K**. Hiding the Elephant in the Room with Experimental Neutrons. Biophys J 119(2): 234-235 (2020)

13. O'Brien ES, Fuglestad B, Lessen HJ, Stetz MA, Lin DW, Marques BS, Gupta, K, Fleming KG, Wand AJ. Membrane Proteins Have Distinct Fast Internal Motion and Residual Conformational Entropy. Angew Chem Int Ed Engl 59(27): 11108-11114 (2020)

14. Ronnebaum TA, **Gupta K**, Christianson DW. Higher-order oligomerization of a chimeric αβγ bifunctional diterpene synthase with prenyltransferase and class II cyclase activities is concentration-dependent. J Struct Biol 210(1): 107463 (2020)

15. Fung HYJ, McKibben KM, Ramirez J, **Gupta K**, Rhoades E. Structural Characterization of Tau in Fuzzy Tau:Tubulin Complexes. Structure 28(3): 378-384.e4, 2020.

16. Arturo EC*, **Gupta K***, Hansen MR, Borne E, Jaffe EK. Biophysical characterization of full-length human phenylalanine hydroxylase provides a deeper understanding of its quaternary structure equilibrium. J Biol Chem 294(26): 10131-10145, 2019. (*=co-first authors)

17. Fugelstad B, **Gupta K**, Wand AJ, Sharp, KA. Water Loading Driven Size, Shape, and Composition of CTAB/hexanol/pentane Reverse Micelles. The Journal of Colloid and Interface Science, Mar 22;540:207-217. doi: 10.1016/j.jcis.2019.01.016. Epub 2019 Jan 6 (2019)

18. Ashkar R, Bilheux HZ, Bordallo HN, Briber RM, Callaway DJE, Cheng X, Chu XQ, Curtis JE, Dadmun M, Fenimore PW, Fushman D, Gabel F, **Gupta K**, Heberle FA, Heinrich F, Hong L, Katsaras J, Kelman Z, Kharlampieva E, Kneller GR, Kovalevsky A, Krueger S, Langan P, Liberman RL, Liu Y, Losche M, Lyman E, Mao Y, Marino JP, Mattos C, Meilleur F, Moody PCE, Nickels JD, O'Neill H, Perez-Salas U, Peters J, Petridis L, Sokolov AP, Wager NJ, Weinrich M, Wymore T, Zhang Y, Smith JC. Progress and Prospects for Neutron Scattering in Biological Sciences. Acta. Cryst. D. Dec 1;74(Pt 12):1129-1168. doi: 10.1107/S2059798318017503. Epub 2018 Dec 20 (2018).

19. Li H, Sharp R, Rutherford K, Gupta, K, Van Duyne GD. Sequence requirements of the Listeria innocua prophage *attP* site. Journal of Molecular Biology Oct 19;430(21):4401-4418. doi: 10.1016/j.jmb.2018.09.007 (2018).

20. Ray-Gallet D, Ricketts MD, Sato Y, **Gupta K**, Boyarchuk E, Senda T, Marmorstein R, Almouzni G.: Functional activity of the H3.3 histone chaperone complex HIRA requires trimerization of the HIRA subunit. Nature Communications 9(1): 3103, August 2018.

21. Gray K, Kaifer K, Baillat D, Wen Y, Bonacci T, Ebert A, Raimer A, Spring A, Have S, Glascock J, **Gupta K**, Van Duyne GD, Emanuele M, Lamond A, Wagner E, Lorson C, Matera AG. Self-oligomerization regulates stability of Survival Motor Neuron (SMN) protein isoforms by sequestering an SCF^{Slmb} degron. Molecular Biology of the Cell, 29(2):96-110. (2017)

22. **Gupta K**, Sharp R, Yuan JB, Li H, Van Duyne GD. Coiled coil Interactions that Mediate Serine Integrase Directionality. Nucleic Acids Research, 45(12):7339-7353 (2017)

23. Mandali S, Dawson AR, **Gupta K**, Van Duyne GD, Johnson RC. Control of Recombination Directionality by the Phage A118 Protein Gp44 and the Coiled-Coil Motif of its Serine Integrase. J. Bacteriol. Mar 13. pii: JB.00019-17. doi: 10.1128/JB.00019-17 (2017)

24. **Gupta K***, Turkki V*, Sherril-Mix S, Hwang Y, Eilers G, Taylor G, McDanal C, Wang P, Temelkoff D, Nolte RT, Velthusien E, Jeffery J, Van Duyne GD, Bushman FD. Structural Basis for Inhibitor-induced Aggregation of HIV Integrase. PLOS Biology http://dx.doi.org/10.1371/journal.pbio.1002584 (2016) (*=co-first authors)

25. Eisemann T, McCauley M, Langelier MF, **Gupta K**, Roy S, Van Duyne GD, Pascal JM. Tankyrase-1 Ankyrin Repeats Form an Adaptable Binding Platform for Targets of ADP-ribose Modification. Structure Sep 1. pii: S0969-2126(16)30225-8 (2016)

26. Arturo EC, **Gupta K**, Heroux A, Stith L, Cross PJ, Parker EJ, Loll PJ, Jaffe EK. The First Structure of Full-Length Mammalian Phenylalanine Hydroxylase Reveals the Architecture of an Auto-Inhibited Tetramer. Proceedings of the National Academy of Sciences Mar 1;113(9):2394-9 (2016)

27. Fuglestad B, **Gupta K**, Wand AJ, Sharp KA. Experimentally Benchmarked Molecular Dynamics Simulations of Cetyl Trimethylammonium Bromide/Hexanol Reverse Micelles. Langmuir Feb 23;32(7):1674-84 (2016)

28. **Gupta K**, Martin R, Sharp R, Sarachan K, Ninan N, Van Duyne GD. Oligomeric properties of SMN•Gemin2 complexes. The Journal of Biological Chemistry Aug 14;290(33):20185-99 (2015)

29. Falk SJ, Guo, LY, Sekulic N, Smoak EM, Mani T, Logsdon G, **Gupta K**, Jansen LET, Van Duyne GD, Vinogradov SA, Lampson MA, Black BE. CENP-C reshapes and stabilizes CENP-A nucleosomes at the centromere. Science 348(6235): 699-703 (2015)

30. Sweeny EA, Jackrel ME, Go MS, Sochor MA, Razzo BM, DeSantis ME, **Gupta K**, Shorter J. The Hsp104 N-terminal domain enables disaggregase plasticity and potentiation. Molecular Cell 57:1-14, (2015)

31. Tao Z, Fusco A, Huang D, **Gupta K**, Ware CF, Van Duyne GD, Ghosh G. p100/IκBδ sequesters and inhibits NF-κB through κBsome formation. Proceedings of the National Academy of Sciences 111(45): 15946-51 (2014)

32. **Gupta K**, Brady T, Dyer B, Hwang Y, Male F, Nolte R, Jeffries J, Van Duyne GD, Bushman FD. Inhibition of Late Replication Steps by an Allosteric Human Immunodeficiency Virus Integrase Inhibitor is Associated with Multimerization of Specific Structural Domains. The Journal of Biological Chemistry 289(30):20477-20488 (2014). **journal cover*

33. **Gupta K**, Contreras LM, Smith D, Qu G, Huang T, Spruce L, Seeholzer S, Belfort M, Van Duyne GD. Quaternary Arrangement of an Active, Native Group II Intron Ribonucleoprotein Complex revealed by Small-angle X-ray Scattering. Nucleic Acids Research 42(8):5347-60 (2014).

34. DeSantis ME, Sweeny EA, Snead D, Leung EH, Go MS, **Gupta K**, Wendler P, Shorter J. Conserved Distal Loop Residues in the Hsp104 and ClpB Middle Domain Contact Nucleotide-Binding Domain 2 and enable Hsp70-Dependent Protein Disaggregation. The Journal of Biological Chemistry 289(2): 848-67 (2014).

35. Martin R, **Gupta K**, Ninan N, Perry K, Van Duyne GD. The Survival of Motor Neurons Protein Forms Soluble Glycine Zipper Oligomers. Structure 20(11):1929-39 (2012).

36. Larue R, **Gupta K**, Wuench C, Shkriabai N, Kessl J, Danhart E, Feng L, Van Duyne GD, Debyser Z, Foster M, Kvaratskhelia M. HIV-1 Integrase C-Terminal Domain Interacts With The Cargo Domain of TNPO3 *in vitro*. The Journal of Biological Chemistry 287(41):34044-58 (2012).

37. **Gupta K**, Curtis J, Krueger S, Hwang Y, Hare S, Cherepanov P, Bushman F, Van Duyne GD. Solution Conformations of Prototype Foamy Virus Integrase and Its Stable Synaptic Complex With U5 viral DNA. Structure 20(11):1918-28 (2012).**featured in Li M and Craigie R, Structure 2012 Nov 7; 20(11):1804-5*

38. Sarachan KL, Valentine KG, **Gupta K**, Moorman VR, Gledhill JM, Bernens, M. Tommos C, Wand AJ, and Van Duyne GD. Solution Structure of the Core SMN-Gemin2 Complex. Biochemical Journal 445(3):361-70 (2012).

39. Devarakonda S, **Gupta K**, Chalmers MJ, Hunt JF, Griffin PR, Van Duyne GD, Spiegelman, BM. Biophysical and Structural Characterization of the Disorder-to-Order Transition in the Metabolic "Hub" PGC-1α upon Complex Assembly with ERRγ. Proceedings of the National Academy of Sciences 108(46):18678-83 (2011).

40. Huang T, Shaikh T, **Gupta K**, Contreras-Martin LM, Grassucci R, Van Duyne GD, Frank J, Belfort M. The Group II Intron Ribonucleoprotein Precursor is a Large, Loosely Packed Structure. Nucleic Acids Research 39(7):2845-2854 (2011). **Featured article (top 5%)*

41. **Gupta K**, Diamond T, Hwang Y, Bushman F, Van Duyne GD. Structural Properties of HIV Integrase-LEDGF Oligomers. The Journal of Biological Chemistry 285(26):20303-20315 (2010).

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Meeting Abstracts:

1. Padilla MS, Shepherd SJ, Hanna A, Kurnik M, Zhang X, Chen M, Mukalel A, Yamagata H, Ricciardi A, Joseph R, Mrksicha K, Siddiquia Z, Issadore D, **Gupta K**, Mitchell MB. Insights into mRNA lipid nanoparticle polydispersity and shape using quantitative solution biophysics. Biomedical Engineering Society Annual Meeting 2024, Baltimore, Maryland.

2. An Z, Lakhani R, Sharp R, **Gupta K**, Van Duyne GD. Expression, Purification, and Biophysical Characterization of Monkeypox Virus Telomere-binding Protein I1. 2024 American Crystallographic Association Meeting, Denver, Colorado.

3. Montermoso S, **Gupta K**, Bushman FD., Van Duyne GD. Understanding the Molecular Mechanism of Redondovirus Rep in Rolling Circle Replication of the Redondoviral Genome. 2024 American Crystallographic Association Meeting, Denver, Colorado.

4. Padilla MS, Shepherd SJ, Hanna A, Kurnik M, Zhang X, Chen M, Mukalel A, Yamagata H, Ricciardi A, Joseph R, Mrksicha K, Siddiquia Z, Issadore D, **Gupta K**, Mitchell MB. Insights into mRNA lipid nanoparticle polydispersity and shape using quantitative solution biophysics. 2024 American Crystallographic Association Meeting, Denver, Colorado.

5. Padilla MS, Shepherd SJ, **Gupta K**, Mitchell MJ. Redefining the Characterization Paradigm of RNA Lipid Nanoparticles. Eastern Analytical Symposium & Exposition 2023. Plainsboro, New Jersey.

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7. Him S, **Gupta K**, Zhou Y, Cui X, Goldman YE, Dantzig JA. mCLIFY: monomeric bright yellow genetically encoded fluorescent protein. 2023 Biophysical Society Meeting. San Diego, California.

8. Eilers G, **Gupta K**, Allen A, Murali H, Sharp R, Hwang Y, Bushman FD, Van Duyne GD. Structure of a Minimal HIV-1 IN-Allosteric Inhibitor Complex at 2.93 Å Resolutions: Routes to Inhibitor Optimization. 2022 American Crystallographic Association Meeting. Portland, Oregon.

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10. Ronnebaum TA, Eaton S, Faylo J, **Gupta K**, Christianson DW. Assembly-line catalysis in bifunctional terpene synthases: (+)-Copalyl diphosphate synthase from fungal *Penicillium* species. Experimental Biology 2022 Meeting, Philadelphia, PA, April 2nd-5th, 2022.

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12. **Gupta K**, Eilers G, Allen A, Montermoso S, Hwang Y, Bushman FD, Van Duyne GD. Structural Insights into Allosteric HIV Integrase Inhibitor Binding and Resistance. 2021 Retrovirus Meeting, Cold Spring Harbor, NY, May 25th-28th, 2021.

13. Eilers G, **Gupta K**, Allen A, Hwang Y, Bushman FD, Van Duyne GD. Influence of the proper amino-terminal sequence on the structure and function of HIV integrase. 2020 Retrovirus Meeting, Cold Spring Harbor, NY, May 18th-23rd, 2020.

14. Arturo EC, Merkel GW, Borne E, Hansen R, Lisowksi S, **Gupta K**, Jaffe E. Amino Acid Substitution at Phe80 of Mammalian Phenylalanine Hydroxylase Destabilizes Both Resting-State and Activated Conformations Increasing the Population of Intermediates. 2020 ASBMB Meeting, San Diego, CA.

15. Ronnebaum TA, **Gupta K**, Christianson DW. Structural and Functional Studies of a Chimeric αβγ Bifunctional Diterpene Synthase with Prenyltransferase and Type II Cyclase Activities. 12th Annual Frontiers in Chemistry and Biology Interface Symposium. Bethesda, Maryland, May 3rd, 2019.

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17. **Gupta K**, Eilers G, Allen A, Giraldo C, Sharp B, Hwang Y, Bushman FD, Van Duyne GD. Higher-order structures of HIV Integrase: Drug-Induced Aggregates of HIV Integrase are Weak Gels. 2019 Retrovirus Meeting, Cold Spring Harbor, NY, May 20th-25th, 2019.

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26. **Gupta K**, Brady T, Dyer BM, Hwang Y, Male F, Nolte RT, Wang L, Velthuisen E, Jeffrey J, Van Duyne GD, and Bushman FD. Linking Inhibition of Late Replication Steps by an Allosteric Inhibitor of Human Immunodeficiency Virus Integrase with Multimerization of Specific Protein Domains. Cold Spring Harbor Retrovirus Meeting, Cold Spring Harbor, N.Y. May 19th-23rd 2014.

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33. Sweeny EA, **Gupta K,** Shorter J. Conformational Changes of HSP104 Revealed Through Small Angle X-Ray Scattering. 2013 Biophysical Society Meeting. Philadelphia, PA. February 3rd -7th 2013.

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Trainees Supervised:

Name	Position/Role	Current Employment/Training
Carolina Giraldo	Research Technician	Medical School, PCOM
Hemma Murali	Research Technician	Graduate Study, University of Pennsylvania
Yara Salim	Research Technician	Graduate Study, Yale University School of Medicine
Cristin McIntosh	Research Technician	Current
Michael Cory	Graduate Rotation Student	Postdoctoral Fellow, Harvard University
Briana Cruga	Graduate Tutorial	Graduate Student (BMB)
Nancy An	Penn Undergraduate (MLS Scholar)	Undergraduate Study, Masters Program Submatriculant
Raju Lakhani	Penn Undergraduate	Undergraduate Study
Nathan Stewart	Penn Undergraduate	Undergraduate Study
Amanda Gore	Penn Undergraduate	Industry
Melanie Reuter	Temple Undergraduate	Graduate Study, U.C. Davis
Nadine Erlazki	Cornell Undergraduate	Graduate Study, Cornell University
Cailean Cavanaugh	Undergraduate	Undergraduate Study
Benjamin Maither	Penn Undergraduate	Undergraduate Study
George Marrah-Walsh	Undergraduate (SUIP)	Graduate Study, Stanford, NSF-GFRP
Liam Bartie	Penn Undergraduate	Research Technician, University of California-Berkeley
Stewart Silver	Penn Undergraduate	
David Nguyen	Penn Undergraduate	Medical School
Jimmy Yuan	Penn Undergraduate	Graduate Study
James Chen	High School, Penn Undergraduate	Postdoctoral Fellow
Wayne Cochran	Undergraduate (SUIP)	Undergraduate Study
Alexander Kang	High School, Penn Undergraduate	Undergraduate Study
Jacob Issac	Penn Undergraduate	Undergraduate Study

Thesis Committees:

Name	Department – Degree	Current Employment/Training
Krystal Haislop	BMB – Ph.D., Completed Dec 2021 (Chair)	Science Writer
Jordan Ontiveros	BMB – Ph.D., Completed June 2022	Industry
Samantha Sustek	BMB – Ph.D. (Chair)	
Leon Palao	BMB – Ph.D.	
Mihyun Oh	Drexel MCBG – Ph.D.	
Andrea Andress	BMB – Ph.D.	

Neha Srikumar	BMB – Ph.D.	
Andy Nguyen	BMB – Ph.D.	