

Michelle Lynn Gill

R&D Manager, NVIDIA Virtual Cell Team

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Currently

I am an R&D Manager on NVIDIA's Virtual Cell team. Our team uses data, deep learning, and HPC to develop models that simulate cellular states. My focus is on the benchmarks and development of supporting tools that help evaluate and improve these models.

Previously I was a Senior Machine Learning Engineer and Data Scientist at BenevolentAI and a member of Arthur Palmer's research group where I developed and applied nuclear magnetic resonance (NMR) spin relaxation experiments to understand how enzyme dynamics are critical to biological function.

Education

Ph.D., Molecular Biophysics & Biochemistry

2003-2006

Yale University, New Haven, CT

Thesis: Development of 205Tl NMR methods for the direct study of monovalent metal ions and ligands in nucleic acids

Advisors: J. Patrick Loria and Scott Strobel

M.Phil., Molecular Biophysics & Biochemistry

2001-2003

Yale University, New Haven, CT

B.S., Biochemistry

1997-2001

University of Kansas, Lawrence, KS

Highest Distinction and Honors (Summa Cum Laude)

Experience

Applied Research Manager, NVIDIA, Virtual Cell Team

2022-Present

Lead benchmarking efforts for virtual cell models, including internal and external collaborations

Developed benchmarking framework and tooling for model assessment and reproducibility

Collaboration with Chan Zuckerberg Initiative on cz-benchmarks for evaluating virtual cell models

Scientific Lead, BioNeMo, NVIDIA

2019-2023

R&D Manager and Scientific Lead for Clara Discovery, NVIDIA's platform for accelerating drug discovery

Developed BioNeMo for pre-training and fine tuning of large language models for cheminformatics and proteomics

Senior AI and Deep Learning Scientist, NVIDIA

2019-2023

Focused on proteomics including deep learning models to predict peptide spectral matches with >95% F1

Led team using GCNNs to predict molecular properties

Senior Data Scientist and Machine Learning Engineer , BenevolentAI	2018-2019
Matrix factorization and GCNNs for drug mechanism importance in knowledge graphs 3D CNNs for ligand pose and affinity prediction	
Senior Deep Learning Consultant , NVIDIA	2017-2018
Assisted clients in pharmaceutical and materials science in utilizing deep learning	
Senior Data Scientist , Metis	2016-2017
Co-instructed 12-week data science bootcamps Developed 12-week machine learning course for F100 company	
Scientist , National Cancer Institute, NIH	2014-2016
Developed parallelized, compressed sensing methods for NMR data reconstruction	
Postdoctoral Research Fellow , Columbia University, Department of Biochemistry and Molecular Biophysics	2008-2014
Demonstrated conformational selection in DNA methyltransferase AlkB Developed multiple quantum NMR spin relaxation experiments Advisor: Professor Arthur G. Palmer, III	
Consultant , The Boston Consulting Group	2006-2007
Worked with clients in finance and pharmaceutical sectors Part of winning team for 2007 Global BCG Strategy Olympics	

Publications

Dicks, S., Heumos, L., Jimenez, S., Angerer, P., Gold, I., Virshup, I., Fischer, F., May, L., Nolet, C. J., Gill, M., Boerries, M., Theis, F. "Accelerating single-cell analysis with GPU-enabled RAPIDS-singlecell." **In preparation** (2025).

Sevgen, E., Moller, J., Lange, A., Parker, J., Quigley, S., Mayer, J., Srivastava, P., Gayatri, S., Hosfield, D., Korshunova, M., Livne, M., Gill, M., Ranganathan, R., Costa, A.B., Ferguson, A.L. "ProT-VAE: Protein transformer variational autoencoder for functional protein design." **Proceedings of the National Academy of Sciences** 122 (2025), doi: 10.1073/pnas.2408737122.

St. John, P., Lin, D., Binder, P., Greaves, M., Shah, V., St. John, J., Lange, A., Hsu, P., Illango, R., Ramanathan, A., Anandkumar, A., Brookes, D.H., Busia, A., Mahajan, A., Malina, S., Prasad, N., Sinai, S., Edwards, L., Gaudet, T., Regep, C., Steinegger, M., Rost, B., Brace, A., Hippe, K., Naef, L., Kamata, K., Armstrong, G., Boyd, K., Cao, Z., Chou, H.Y., Chu, S., dos Santos Costa, A., Darabi, S., Dawson, E., Didi, K., Fu, C., Geiger, M., Gill, M., Hsu, D.J., Kaushik, G., Korshunova, M., Kothen-Hill, S., Lee, Y., Liu, M., Livne, M., McClure, Z., Mitchell, J., Moradzadeh, A., Mosafi, O., Nashed, Y., Paliwal, S., Peng, Y., Rabhi, S., Ramezanghorbani, F., Reidenbach, D., Ricketts, C., Roland, B.C., Shah, K., Shimko, T., Sirelkhathim, H., Srinivasan, S., Stern, A.C., Toczydlowska, D., Veccham, S.P., Venanzi, N.A.E., Vorontsov, A., Wilber, J., Wilkinson, I., Wong, W.J., Xue, E., Ye, C., Yu, X., Zhang, Y., Zhou, G., Zandstein, B., Chacon, A., Sohani, P., Stadler, M., Hundt, C., Zhu, F., Dallago, C., Trentini, B., Kucukbenli, E., Rvachov, T., Calleja, E., Israeli, J., Clifford, H., Haukioja, R., Haemel, N., Tretina, K., Tadimetri, N., Costa, A.B..

"BioNeMo Framework: a modular, high-performance library for AI model development in drug discovery." **arXiv** (2024), doi: 10.48550/arXiv.2411.10548.

Strauss, M.T., Bludau, I., Zeng, W.F., Voytik, E., Ammar, C., Schessner, J., Illango, R., Gill, M.L., Meier, F., Willems, S., Mann, M.. "AlphaPept, a modern and open framework for MS-based proteomics." **Nature Communications** 15 (2024), doi: 10.1038/s41467-024-46485-4.

Gill, M.L.. "The rise of the machines in chemistry." **Magnetic Resonance in Chemistry** 60, 1044–1051 (2022), doi: 10.1002/mrc.5304.

Reidenbach, D., Livne, M., Illango, R.K., Gill, M.L., Israeli, J.I.. "Improving small molecule generation using mutual information machine." **arXiv** (2022), doi: 10.48550/arXiv.2208.09016.

Gill, M.L., Hsu, A., Palmer, A.G.. "Detection of chemical exchange in methyl groups of macromolecules." **Journal of Biomolecular NMR** 73, 443–450 (2019), doi: 10.1007/s10858-019-00240-w.

Tong, M., Pelton, J., Gill, M.L., Zhang, W., Picart, F., Seeliger, M.. "Survey of solution dynamics in Src kinase reveals cross talk between the ligand binding and regulatory sites." **Nature Communications** 8, 2160 (2017), doi: 10.1038/s41467-017-02240-6.

Gill, M.L., Byrd, R.A., Palmer, A.G.. "Dynamics of GCN4 facilitate DNA interaction: a model-free analysis of an intrinsically disordered region." **Physical Chemistry and Chemical Physics** 18, 5839–5849 (2016), doi: 10.1039/c5cp06197k.

Sun, S., Gill, M.L., Li, Y., Huang, M., Byrd, R.A.. "Efficient and generalized processing of multidimensional NUS NMR data: the NESTA algorithm and comparison of regularization terms." **Journal of Biomolecular NMR** 62, 105–117 (2015), doi: 10.1007/s10858-015-9923-x.

Gill, M.L., Palmer, A.G.. "Local isotropic diffusion approximation for coupled internal and overall molecular motions in NMR spin relaxation." **Journal of Physical Chemistry B** 118, 11120–11128 (2014), doi: 10.1021/jp506580c.

Gill, M.L., Byrd, R.A.. "Dynamic activation of apoptosis: conformational ensembles of cIAP1 are linked to a spring-loaded mechanism." **Nature Structural Molecular Biology** 21, 1022–1023 (2014), doi: 10.1038/nsmb.2925.

Ergel, B., Gill, M.L., Brown, L., Yu, B., Palmer, A.G., Hunt, J.F.. "Protein dynamics control the progression and efficiency of the catalytic reaction cycle of AlkB." **Journal of Biological Chemistry** 289, 29584–29601 (2014), doi: 10.1074/jbc.M114.575647.

Gill, M.L., Palmer, A.G.. "Multiplet-filtered and gradient-selected zero-quantum TROSY experiments for ¹³C¹H³ methyl groups in proteins." **Journal of Biomolecular NMR** 51, 245–251 (2011), doi: 10.1007/s10858-011-9533-1.

Ramsey, J.D., Gill, M.L., Kamerzell, T.J., Price, E.S., Joshi, S.B., Bishop, S.M., Oliver, C.N., Middaugh, C.R.. "Using empirical phase diagrams to understand the role of intramolecular dynamics in immunoglobulin

G stability." **Journal of Pharmaceutical Sciences** 98, 2432–2447 (2009), doi: 10.1002/jps.21619.

Gill, M.L., Strobel, S.A., Loria, J.P.. "Crystallization and characterization of the thallium form of the Oxytricha nova G-quadruplex." **Nucleic Acids Research** 34, 4506–4514 (2006), doi: 10.1093/nar/gkl616.

Beach, H., Cole, R., Gill, M.L., Loria, J.P.. "Conservation of μ s-ms enzyme motions in the apo- and substrate-mimicked state." **Journal of the American Chemical Society** 127, 9167–9176 (2005), doi: 10.1021/ja0514949.

Gill, M.L., Strobel, S.A., Loria, J.P.. "205Tl NMR methods for the study of monovalent metal binding sites in nucleic acids." **Journal of the American Chemical Society** 127, 16723–16732 (2005), doi: 10.1021/ja055358f.

Adams, P.L., Stahley, M.R., Gill, M.L., Kosek, A.B., Wang, J., Strobel, S.A.. "Crystal structure of a group I intron splicing intermediate." **RNA** 10, 1867–1887 (2004), doi: 10.1261/rna.7140504.

Wiethoff, C.M., Gill, M.L., Koe, G.S., Koe, J.G., Middaugh, C.R.. "A fluorescence study of the structure and accessibility of plasmid DNA condensed with cationic gene delivery vehicles." **Journal of Pharmaceutical Sciences** 92, 1272–1285 (2003), doi: 10.1002/jps.10391.

Wiethoff, C.M., Gill, M.L., Koe, G.S., Koe, J.G., Middaugh, C.R.. "The structural organization of cationic lipid-DNA complexes." **Journal of Biological Chemistry** 277, 44980–44987 (2002), doi: 10.1074/jbc.M207758200.

Silchenko, S., Sippel, M.L., Kuchment, O., Benson, D.R., Mauk, A.G., Altuve, A., Rivera, M.. "Hemin is kinetically trapped in cytochrome b5 from rat outer mitochondrial membrane." **Biochemical and Biophysical Research Communications** 273, 467–472 (2000), doi: 10.1006/bbrc.2000.2968.

Patents

Automated FEP Path Generation and Optimization by Molecule Foundation Models and Generative AI	2025
Peng, Y., Kucukbenli, E., Zhou, G., Gill, M.L., Livne, M., Korshunova, M., Rvachov, T., Israeli, Y.	
US Patent Application No. 19/208,119; Filing Date: 2025/05/14	
Extraction of Informative Embeddings from Encoder-Decoder Models	2024
Livne, M., Gill, M.L.	
US Patent Application No. 18/957,301; Filing Date: 2024/11/22	
Contrastive Framework for Unified Generative and Discriminative Representation Learning	2024
Livne, M., Gill, M.L.	
US Patent Application No. 18/957,294; Filing Date: 2024/11/22	
Efficient Data Loading for Deep Learning Workloads	2024
Darabi, S., Korshunova, M., Grewal, J., Gill, M.L., Morkisz, P.	
US Patent Application No. 18/885,428; Filing Date: 2024/09/13	

Guardrails for Molecular Generation	2024
Korshunova, M., Peng, Y., Zhou, G., Rvachov, T., Gill, M.L., Kucukbenli, E., Israeli, Y. US Patent Application No. 18/807,805; Filing Date: 2024/08/16	
Guardrails for Conditional Molecular Generation	2024
Korshunova, M., Peng, Y., Zhou, G., Rvachov, T., Gill, M.L., Kucukbenli, E., Israeli, Y. US Patent Application No. 18/807,808; Filing Date: 2024/08/16	
Training-Time Guardrails for Molecular Generation	2024
Korshunova, M., Peng, Y., Zhou, G., Rvachov, T., Gill, M.L., Kucukbenli, E., Israeli, Y. US Patent Application No. 18/807,811; Filing Date: 2024/08/16	
Guardrails for Instruction-Tuned Molecular Generation	2024
Korshunova, M., Peng, Y., Zhou, G., Rvachov, T., Gill, M.L., Kucukbenli, E., Israeli, Y. US Patent Application No. 18/807,814; Filing Date: 2024/08/16	
End to End Deep Learning Workflow for In Silico Molecule Design	2024
Stern, A., Gill, M.L., Stepniewska-Dziubinska, M., Grzegorzec, T., Nowaczynski, A., Toczydlowska, D., Israeli, Y., Ribalta Lorenzo, P. US Patent Application No. 18/412,168; Filing Date: 2024/01/12	
Small Molecule Generation Using Machine Learning Models	2023
Livne, M., Reidenbach, D., Gill, M.L., Ilango, R., Israeli, Y. US Patent Application No. 18/450,745; Filing Date: 2023/08/16	

Presentations

Scientific Discovery: From the Lab Bench to the GPU , Andy Byrd Retirement Symposium Invited Keynote, April 19, 2024, Institute for Bioscience & Biotechnology Research, University of Maryland, NIST, Bethesda, MD Slides · Program	2024
Scientific Discovery: From the Lab Bench to the GPU , PyData NYC Invited Keynote, November 2, 2023, New York, NY Slides · Video · Abstract	2023
NVIDIA BioNeMo: A framework and service for development and use of generative AI in drug discovery , 6th RSC-BMCS / RSC-CICAG Artificial Intelligence in Chemistry Conference Invited Keynote, September 5, 2023, Cambridge, UK Slides · Program	2023
Exploring Molecular Space and Accelerating Drug Discovery on the GPU with Clara Discovery , Gates Foundation Grand Challenges: Applications of Artificial Intelligence in Machine Learning Invited Talk, November 10, 2021, Virtual	2021
Accelerating Drug Discovery with Clara Discovery and MegaMolBART , 4th RSC-BMCS / RSC-CICAG Artificial Intelligence in Chemistry Invited Talk, September 27, 2021, Virtual Slides	2021

Real Time, GPU-Accelerated Analysis and Visualization in the Life Sciences , Ken Kennedy Institute Data Science Conference Michelle Gill and Avantika Lal Invited Keynote, October 26-27, 2020, Virtual Slides · Abstract · Program	2020
Artificial intelligence driven drug discovery , NYC R Conference Invited Presentation, May 10, 2019, New York, NY Slides	2019
Panel: Careers in data science , Tri-Institutional Career Symposium April 9, 2019, Memorial Sloan Kettering Cancer Center, The Rockefeller University and Weill Cornell Medicine, New York, NY Program	2019
Machine learning for target identification and lead optimization in drug discovery , New York Area Group for Informatics and Modeling Alix Lacoste and Michelle Gill Invited Presentation, February 26, 2019, New York, NY Abstract	2019
Accelerating the journey from data to medicine , NeurIPS Amir Saffari, Dan Neil, Alix Lacoste, and Michelle Gill Expo Talk, 2018, Montreal, Canada Abstract	2018
Artificial intelligence as a catalyst for scientific discovery , JupyterCon Invited Keynote, 2018, New York, NY Slides · Video · Abstract	2018
From structural biology to AI: a holistic approach to studying molecular machines , Brookhaven National Laboratory Invited Presentation, 2018, Upton, NY Slides	2018
Efficient image search and identification: the making of Wine-O.AI , SciPy Conference Selected Presentation, 2017, Austin, TX Slides · Video · Code	2017
Development of 2D/3D NMR methods for the direct study of monovalent metal ions and ligands in nucleic acids , Ph.D. Thesis Defense, Yale University 2006, New Haven, CT Slides · Thesis	2006

Awards

NIH Postdoctoral Research Fellowship (F32 GM089047)	2009-2012
Global BCG Strategy Olympics, Winning Team	2007
NSF Graduate Research Fellowship	2002-2006

	Barry M. Goldwater Scholar	2000-2001
	Outstanding Undergraduate Honors Research Thesis	2001
	Kansas Board of Regents Full Tuition Merit Scholarship	1997-2001
Service	Judge, Preliminary and Final Rounds , NYC STEM Fair, New York, NY Evaluated submissions in the biochemistry track	2022
	Program Chair , PyData NYC, New York, NY Responsible for conference content, proposal review, speaker selection, and scheduling	2018
	Machine Learning Symposium Co-Chair , SciPy Conference, Austin, TX Co-chair of machine learning / deep learning symposium	2018
	Proposal Reviewer , JupyterCon	2018
	Reviewer , Journal of Open Source Software (JOSS)	2018-2019