

# Michelle Lynn Gill, PhD

Applied Research Manager, NVIDIA Virtual Cell Team

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## Overview

I am an Applied Research 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

<b>Ph.D., Molecular Biophysics &amp; Biochemistry</b>	2003-2006
Yale University, New Haven, CT	
Thesis: Development of $^{205}\text{TI}$ NMR methods for the direct study of monovalent metal ions and ligands in nucleic acids	
Advisors: J. Patrick Loria and Scott Strobel	
<b>M.Phil., Molecular Biophysics &amp; Biochemistry</b>	2001-2003
Yale University, New Haven, CT	
<b>B.S., Biochemistry</b>	1997-2001
University of Kansas, Lawrence, KS	
Highest Distinction and Honors (Summa Cum Laude)	

## Experience

<b>Applied Research Manager</b> , 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	
<b>Scientific Lead, BioNeMo</b> , 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	
<b>Senior AI and Deep Learning Scientist</b> , 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

**Scientist,** National Cancer Institute, NIH

2014-2016

Developed parallelized, compressed sensing methods for NMR data reconstruction

**Postdoctoral Research Fellow,** Columbia University, Department of

2008-2014

Biochemistry and Molecular Biophysics

Demonstrated conformational selection in DNA methyltransferase AlkB

Developed multiple quantum NMR spin relaxation experiments

Advisor: Professor Arthur G. Palmer, III

**Publications**

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

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

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

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

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

D. Reidenbach, M. Livne, R.K. Illango, M.L. Gill, and J.I. Israeli "Improving small molecule generation using mutual information machine" arXiv (2022).

M.L. Gill, A. Hsu, and A.G. Palmer "Detection of chemical exchange in methyl groups of macromolecules" Journal of Biomolecular NMR (2019).

M.L. Gill, R.A. Byrd, and A.G. Palmer "Dynamics of GCN4 facilitate DNA interaction: a model-free analysis of an intrinsically disordered region" Physical Chemistry and Chemical Physics (2016).

S. Sun, M.L. Gill, Y. Li, M. Huang, and R.A. Byrd "Efficient and generalized processing of multidimensional NUS NMR data: the NESTA algorithm and comparison of regularization terms" Journal of Biomolecular NMR (2015).

B. Ergel, M.L. Gill, L. Brown, B. Yu, A.G. Palmer, and J.F. Hunt "Protein dynamics control the progression and efficiency of the catalytic reaction cycle of AlkB" Journal of Biological Chemistry (2014).

M.L. Gill, and A.G. Palmer "Local isotropic diffusion approximation for coupled internal and overall molecular motions in NMR spin relaxation" Journal of Physical Chemistry B (2014).

M.L. Gill, and A.G. Palmer "Multiplet-filtered and gradient-selected zero-quantum TROSY experiments for <sup>13</sup>C<sup>1</sup>H<sub>3</sub> methyl groups in proteins" Journal of Biomolecular NMR (2011).

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

**End to End Deep Learning Workflow for In Silico Molecule Design** 2024

Stern, A., Gill, M.L., Stepniewska-Dziubinska, M., Grzegorzek, 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 2024

Retirement Symposium

Invited Keynote, April 19, 2024, Institute for Bioscience & Biotechnology Research,  
University of Maryland, NIST, Bethesda, MD

[Slides](#) · [Program](#)

**Scientific Discovery: From the Lab Bench to the GPU**, PyData NYC 2023

Invited Keynote, November 2, 2023, New York, NY

[Slides](#) · [Video](#) · [Abstract](#)

**NVIDIA BioNeMo: A framework and service for development and** 2023

**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](#)

**Exploring Molecular Space and Accelerating Drug Discovery on** 2021

**the GPU with Clara Discovery**, Gates Foundation Grand Challenges: Applications of Artificial Intelligence in Machine Learning

Invited Talk, November 10, 2021, Virtual

**Accelerating Drug Discovery with Clara Discovery and** 2021

**MegaMolBART**, 4th RSC-BMCS / RSC-CICAG Artificial Intelligence in Chemistry

Invited Talk, September 27, 2021, Virtual

[Slides](#)

**Real Time, GPU-Accelerated Analysis and Visualization in the Life Sciences**, Ken Kennedy Institute Data Science Conference 2020

Michelle Gill and Avantika Lal

Invited Keynote, October 26-27, 2020, Virtual

[Slides](#) · [Abstract](#) · [Program](#)

## **Artificial intelligence driven drug discovery**, NYC R Conference

2019

Invited Presentation, May 10, 2019, New York, NY

[Slides](#)

## **Machine learning for target identification and lead optimization in drug discovery**, New York Area Group for Informatics and Modeling

2019

Alix Lacoste and [Michelle Gill](#)

Invited Presentation, February 26, 2019, New York, NY

[Abstract](#)

## **Accelerating the journey from data to medicine**, NeurIPS

2018

Amir Saffari, Dan Neil, Alix Lacoste, and [Michelle Gill](#)

Expo Talk, 2018, Montreal, Canada

[Abstract](#)

## **Artificial intelligence as a catalyst for scientific discovery**,

2018

JupyterCon

Invited Keynote, 2018, New York, NY

[Slides](#) · [Video](#) · [Abstract](#)

## **From structural biology to AI: a holistic approach to studying molecular machines**, Brookhaven National Laboratory

2018

Invited Presentation, 2018, Upton, NY

[Slides](#)

## **Efficient image search and identification: the making of Wine-O.AI**, SciPy Conference

2017

Selected Presentation, 2017, Austin, TX

[Slides](#) · [Video](#) · [Code](#)

## **Development of $^{205}\text{TI}$ NMR methods for the direct study of monovalent metal ions and ligands in nucleic acids**, Ph.D. Thesis Defense, Yale University

2006

Thesis Defense, 2006, New Haven, CT

[Slides](#) · [Thesis](#)

## 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,

2022

NY

Evaluated submissions in the biochemistry track

**Program Chair**, PyData NYC, New York, NY

2018

Responsible for conference content, proposal review, speaker selection, and scheduling

**Machine Learning Symposium Co-Chair**, SciPy Conference, Austin,

2018

TX

Co-chair of machine learning / deep learning symposium