

# MARTIN WEISS

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EDUCATION	<b>Virginia Tech</b>	Blacksburg, Virginia
	<b>M.S. Computer Engineering</b>	2024 – 2026
	<b>B.S. Computer Engineering</b>	2020 – 2024
	Major: Machine Learning, <i>Cum Laude</i>	
EXPERIENCE	<b>Data Science Co-Op</b>	Rahway, NJ
	<b>Merck Research Laboratories</b>	January 2025 – Present
	Member of Screening and Compound Profiling Group as a Computational Data Scientist	
	Working on custom models for virtual screening and hit-picking	
	Developed transformer-based diffusion model for small molecule conformer generation	
	Leveraging terabytes of chemical data to build foundational models for virtual screening	
	Training large-scale models using a multi-node HPC environment with NVIDIA GPUs	
	<b>Student Researcher</b>	Blacksburg, VA
	<b>Virginia Tech National Security Institute</b>	September 2024 – December 2024
	Leveraged YOLOv7 to detect wireless signals from spectrogram images	
	Developed custom YOLOv7 based models to maintain spatial alignment of input images	
	Extracted features from detected signals for further analysis	
	Applied UMAP for dimensionality reduction and outlier detection from extracted features	
	<b>Senior Data Science Intern</b>	Guilford, CT
	<b>Thermo Fisher Scientific</b>	May 2024 – August 2024
	Worked on various deep learning projects with NGS R&D engineering group	
	Fine-tuned FLAN-T5 LLM to create dictionaries from sequencing workflow comments	
	Developed models using PyTorch to predict 2D histograms using sequencing run metadata	
	Achieved >99% accuracy in identifying the 0.25% of sequencing runs that were aberrant	
	Utilized NVIDIA GPUs and CUDA to accelerate model training and inferencing	
	<b>Data Science Intern</b>	Kalamazoo, MI
	<b>Thermo Fisher Scientific</b>	May 2023 – August 2023
	Led a data-driven targeting for diagnostic tests within ImmunoDiagnostics	
	Created machine learning models to identify test utilization drivers among physicians	
	Engineered targeting algorithms that aligned with business objectives for demand generation	
	<b>Data Science Intern</b>	Washington, D.C.
	<b>Municipal Securities Rulemaking Board</b>	May 2022 – July 2022
	Developed machine learning solutions to analyze and predict bond report filing times	
	Created data visualizations and graphs that promoted explainability and interpretability	
SKILLS	<b>Languages:</b> Python, Bash, SQL, R, L <sup>A</sup> T <sub>E</sub> X	
	<b>Machine Learning &amp; Deep Learning:</b> PyTorch, TensorFlow, Keras, scikit-learn, OpenCV	
	<b>Cheminformatics:</b> RDKit, OEChem TK	
	<b>Data Manipulation:</b> pandas, NumPy, Polars	
	<b>Visualization:</b> Plotly, seaborn, py3Dmol, PyMOL	
	<b>Tools:</b> AWS, PBS Pro, Docker, CUDA, Jupyter, Git, Ubuntu	