
PROFESSIONAL SUMMARY

- Structural biologist and biochemist with 20+ years of experience across academia and biotech R&D.
- Expert in transcription mechanisms from bacteria to humans and structure-guided drug design in oncology and inflammation.
- Directed multidisciplinary projects while remaining hands-on in experimental and computational work.

CORE EXPERTISE

Computational chemistry and structure-based drug design: Schrödinger Suite (docking/IFD-MD, MD/ensemble analysis, FEP+, WaterMap); RDKit; ligandability assessment; covalent inhibitor design; cheminformatics for chemical-space exploration and scaffold hopping; multiparameter optimization in LiveDesign

Structural and experimental biology: X-ray crystallography; cryo-EM; protein expression and purification; protein-protein and protein-nucleic acid interaction analysis; biochemical assay development; stopped-flow kinetics; SELEX

Discovery strategy and program leadership: target tractability; chemotype and hit-to-lead strategy; SAR and assay data interpretation

AI and scientific computing: Python; structural bioinformatics (sequence/MSA analysis, evolutionary covariance, structural alignment, protein interaction interface mapping); AI-assisted coding and data analysis; hierarchical multi-agent workflows; large-scale AlphaFold 3 modeling; integration of structural and functional datasets; HPC

PROFESSIONAL EXPERIENCE

STANFORD UNIVERSITY SCHOOL OF MEDICINE | Palo Alto, CA

2021-Present

Senior Research Engineer (2022-Present) | Visiting Scholar (2021-2022), Roger D. Kornberg Laboratory

- Developed a mechanistic model of how activator engagement of human Mediator influences RNA polymerase II initiation. An initial version appeared in a 2025 perspective; the full study is now submitted.
- Built an end-to-end computational pipeline integrating large-scale AlphaFold 3 co-folding with structural and functional datasets to map recurrent activator interactions with human Mediator. Designed AI reasoning infrastructure around an Obsidian project knowledge base and hierarchical Claude Code/Codex workflows for scripting, result review, and adversarial hypothesis testing.
- Published a single-author Trends Biochem. Sci. perspective (2024) proposing a unified mechanistic framework for promoter melting.

INTERX / NEOTX, LAB DIVISION | Menlo Park, CA

2019-2023

Scientific Director & Head of Biology (2019-2022) | Scientific Director / Consultant, part-time (2022-2023)

- Led structure-guided strategy for PD-L1 small-molecule discovery (manuscript in preparation), and worked on PARP and TNF- α .
- Advanced PD-L1 chemistry from a fragment hit to a differentiated lead series with low-nanomolar biochemical activity and a binding mode confirmed by X-ray crystallography, establishing a novel chemotype in a patent-crowded inhibitor landscape. Expanded into sp³-enriched ligand space using custom cheminformatics scripting.
- Set compound-prioritization and follow-up design priorities by weighing structural models, SAR, and biochemical/cellular assay data.
- Worked with Robert Dow (BioPharmaWorks; Pfizer veteran) and Stevan Djuric (former AbbVie VP, Discovery Chemistry) as senior medicinal chemistry advisors, providing independent structure-guided input on design decisions.
- Led a five-person MS/PhD discovery team, coordinated external consultants and CROs, and contributed to target selection, scientific hiring, and IP strategy, including provisional patent preparation.

ROCKEFELLER UNIVERSITY | New York, NY

2006-2019

Research Associate/ Independent Project Lead (2011-2019) | Postdoctoral Fellow (2006-2011), Seth A. Darst Laboratory

- Designed and executed structural and mechanistic studies of bacterial transcription using X-ray crystallography, single-particle cryo-EM, reconstituted transcription biochemistry, and stopped-flow fluorescence kinetics.
- Defined key structural and kinetic principles of bacterial promoter recognition and transcription-bubble formation, culminating in a *Cell* cover article (first/co-corresponding author) and a *Science* paper (first/corresponding author).

ADDITIONAL DRUG DISCOVERY & TARGET-STRATEGY PROGRAMS

PARP: Defined an initial structure-based approach centered on the adenine pocket, assessing existing chemical matter, assay feasibility, and target tractability.

TNF- α : Developed a novel small-molecule strategy informed by structural analysis and disease rationale; contributed to a successful Israel Innovation Authority grant application.

AHR / inflammatory bowel disease (IBD): Advised an early-stage startup on AHR target evaluation in chronic IBD, assessing receptor biology, ligand selectivity, and disease relevance.

ADDITIONAL RESEARCH EXPERIENCE

UNIVERSITY OF WISCONSIN-MADISON | Madison, WI

2014

Honorary Fellow, Robert C. Landick Laboratory

- Used stopped-flow fluorescence kinetics and a panel of conformation-selective antibiotics to resolve RNA polymerase dynamics during promoter opening.

PUBLIC HEALTH RESEARCH INSTITUTE | Newark, NJ

2004-2006

Research Scientist, Alexander D. Goldfarb Laboratory

- Clarified a key mechanistic question in the action of rifampicin, a clinically important first-line tuberculosis antibiotic; published as first author in PNAS.

INSTITUTE OF MOLECULAR GENETICS / MOSCOW STATE UNIVERSITY | Moscow, Russia

2002-2006

Graduate Researcher, Andrey V. Kulbachinskiy Laboratory

- Used SELEX and mechanistic biochemistry to identify high-affinity RNA polymerase aptamers and discover a previously unrecognized bacterial promoter element (first author in *Molecular Cell*).

SELECTED PUBLICATIONS & MANUSCRIPTS

Author key: underlined name = first author; * = corresponding author.

Submitted

- Feklistov A*, Kornberg RD. [A Structural Model of Transcriptional Activation by Mediator](#). bioRxiv (2026). doi: 10.64898/2026.10.01.756097.

In preparation

- Feklistov A*, et al. Structure-Guided Design of Phenyl-Benzothiophene and sp³-Enriched Spirocyclic PD-L1 Dimerization Inducers.

Published

- Kornberg RD, Feklistov A*. In Defense of Biochemistry: Studies of Transcriptional Regulation. *Journal of Molecular Biology*. 2025;437(22):169299.
- Feklistov A*. Dynamics and logic of promoter melting. *Trends in Biochemical Sciences*. 2024;49:8-11.
- Feklistov A*, et al. RNA polymerase motions during promoter melting. *Science*. 2017;356:863-866.
- Bae B, Feklistov A, et al. Structure of a bacterial RNA polymerase holoenzyme open promoter complex. *eLife*. 2015;4:e08504. Equal contribution.
- Feklistov A*, Darst SA. Structural basis for promoter -10 element recognition by the bacterial RNA polymerase sigma subunit. *Cell*. 2011;147:1257-1269. **Cover story**.
- Feklistov A, et al. Rifamycins do not function by allosteric modulation of Mg²⁺ binding to the RNA polymerase active center. *PNAS*. 2008;105:14820-14825.
- Feklistov A, et al. A basal promoter element recognized by free RNA polymerase sigma subunit determines promoter recognition by RNA polymerase holoenzyme. *Molecular Cell*. 2006;23:97-107.

Full publication record: [Google Scholar](#)

SELECTED TALKS

- Invited seminars:** Karolinska Institute (2018); University of Birmingham (2018); Hong Kong University of Science and Technology (2014).
- Selected conference talks:** Harden Conference, "Machines on Genes IV" (2016); FASEB SRC Mechanism and Regulation of Prokaryotic Transcription (2015, 2011); Gordon Research Conference, Nucleic Acids (2015).

EDUCATION & SELECTED TRAINING

PhD, Molecular Biology | Moscow State University, 2006

BSc/MS, Biochemistry, summa cum laude | Moscow State University, 2002

Selected training: Medicinal Chemistry in Drug Discovery (Drew University); High-Throughput Virtual Screening (Schrödinger); X-Ray Methods in Structural Biology (CSHL); RapiData X-Ray Crystallography (NLS/Brookhaven); CCP4 Crystallography School (APS/Argonne); stopped-flow kinetics workshop (UT Austin); Stanford AI training.

SELECTED HONORS & PROFESSIONAL SERVICE

- [Blavatnik Award for Young Scientists](#) (2012)
- [Merck Foundation Postdoctoral Fellowship](#) (2009-2011)
- [Evrogen JSC Award for Young Scientists](#) (2002)
- [International Biology Olympiad Silver Medal](#) (1997)

Ad hoc reviewer: Science, Nature Reviews Microbiology, Genes & Development, Cell Reports, Biochemistry, BMC Biology, and Journal of Molecular Biology.