Marc C. Deller, D Phil

Research Fellow | Molecular Science Expertise | Drug Discovery Leadership & Innovation

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SUMMARY

An entrepreneurial and innovative molecular sciences professional with over 20 years of leadership experience in protein science and drug discovery. Expert in X-ray crystallography, Cryo-EM, new modalities, and hit-to-lead strategies. My key achievements include establishing a state-of-the-art $8M automated structural biology platform and determining over 400 complex protein structures, contributing to 6 preclinical FDA IND submissions, and accelerating structural biology workflows by 4-fold. Synthesized insights from emerging technologies and adjacent scientific fields to create actionable proposals that expand the R&D pipeline and foster external innovation partnerships. I'm seeking a position where my drug discovery leadership and cross-functional collaboration skills can be leveraged to support your mission of advancing transformative innovations in therapeutic development.

EXPERIENCE

Research Fellow

Incyte Pharmaceuticals, Structural Biology - 2 Years, 10 months

03/2022 - 12/2024 Wilmington, United States

- Determined over **100** challenging co-crystal structures for medicinal and computational chemistry teams, conducted SBDD and FBDD analysis for **10+** oncology and immunology programs. Accelerated hit-to-lead processes and improved ADME/DMPK profiles for rapid bench-to-clinic.
- Implemented innovative experimental approaches, including advanced cloud and hardware capabilities. Reduced timelines by **67%** using automated liquid handling, imaging, AI/ML, sample tracking, cloud computing, and accelerated data strategy.
- Identified **5** new protein targets using computational chemistry, tractability and "druggability" workflows, and validation of protein co-complexes.
- Managed external CRO capabilities to expand screening capabilities via **5+** collaborations to enable protein production, Fragment-Based Drug Discovery, NMR, WAC, and validation of protein co-complexes.
- Supported **3** FDA IND filings, **3** patent applications, and **3** manuscripts.
- Contributed to the discovery of **4** new oncology and immunology leads for previously "undruggable" targets. Utilized structural, biophysical and protein characterization techniques, including DLS/DFS/Massphotometry to characterize new biologics, small molecules, and cell therapies.

Associate Director

Incyte Pharmaceuticals, Structural Biology - 4 years, 1 month

03/2018 - 03/2022 Wilmington, United States

- Established an **$8M** automated state-of-the-art structural biology platform, from the ground up, featuring X-ray crystallography and Cryo-EM.
- Overcame protein production, synchrotron data, and CryoEM data collection bottlenecks by developing internal/external capabilities including **10+** external CROs.
- Managed a team of **10+** scientists in a matrixed environment and coordinated research efforts across **10+** oncology programs, streamlined platform and infrastructure operations, and budgets **$1.5M+.**

Director

Stanford University, Macromolecular Structure Knowledge Center - 2 years, 10 months

06/2015 - 03/2018 California, United States

- Directed the design and implementation of a new structural biology service center, managing budgets of **$1M** and facilitating access for over **50** SSRL/SLAC users.
- Supervised a team of **2** scientists and guided **50+** users in the utilization of high-throughput platforms.
- Generated user base, resulting in **10** new SSRL/SLAC users, **6** novel protein structures, **2** peer-reviewed publications, **3** grant applications, and approximately **$60,000** revenue.
- Organized and led campus-wide training of Schrödinger computational platform to over **50** users.

MY PHILOSOPHY

Curiosity: 20 years leading innovations in protein structure and drug discovery, identifying and integrating emerging scientific breakthroughs to enrich R&D pipelines and guide over **20** oncology and immunology programs. Produced platforms and strategic white papers, and led open innovation and program governance for board-level review and strategic alignment.

Courage: 400 complex protein structures determined using X-ray and CryoEM in top academic and industry settings, overcoming scientific barriers and enabling breakthroughs for "undruggable" targets. Launched **2** research platforms, drove adoption of biotech-inspired models, and enabled transformative innovations and organizational change.

Creativity: 3 patents and numerous key discoveries in immunology, HIV, and cancer, pioneering novel biologic, antibody, and small molecule strategies. Designed and led ideation workshops and innovation sprints to scale high-impact scientific programs and address unmet medical needs.

Communication: 60+ manuscripts published on protein structures—including cytokines, receptors, kinases, membrane proteins, biologics, and antibodies—and delivered innovation-focused reports and presentations. Developed KPIs and frameworks to measure and communicate scientific impact across teams.

Compassion: 6 preclinical FDA INDs approved and advanced to help cancer patients in need, translating foundational science into potential therapies. Mentored cross-functional teams of **50+** and chaired proposal committees to drive patient-focused solutions.

Collaboration: 2 state-of-the-art automated X-ray and Cryo-EM labs established from the ground up, managing **$8M+** budgets. Led cross-functional and external partnerships at the interface of biology, chemistry, biophysics, and AI to accelerate discovery, data strategy, and translational solutions.

EXPERTISE

Structural Biology Leadership

Gene-to-Structure expertise, led structural biology efforts for drug discovery programs, leveraging refinement and data processing expertise in X-ray crystallography, Cryo-EM, NMR, and AI-driven design.

Advanced Protein & Molecular Science

Expert in molecular sciences, molecular biology, construct design, protein expression, purification, structure-function analysis, and structure validation. Skilled in SAR, biophysical characterization, and data analytics to validate protein interactions and communicate complex concepts.

EXPERIENCE

Senior Scientist

Scripps Research Institute, Joint Center for Structural Genomics - 8 years, 11 months

08/2006 - 06/2015 San Diego, United States

- Developed automated crystallography-based sample prep, data collection, and gene-to-structure workflows as part of large-scale NIH sponsored Protein Structure Initiative.
- Enhanced structural genomics success rates by 10% through workflow optimization, process automation, and target salvage pathways.
- Authored/co-authored over 40 peer-reviewed manuscripts and determined over 70 novel protein structures including membrane proteins, and HIV receptors targeting cell therapies for immunology and oncology.

Principal Scientist

Pfizer, Structural Biology - 4 years, 6 months

08/2001 - 01/2006 San Diego, United States

- Led crystallography-based SBDD pipelines, sample prep, data collection, and protein co-complex validation.
- Determined over 200 protein structures, advancing global drug discovery initiatives across Pfizer labs.
- Guided global chemistry, computational chemistry, computational science, data, and clinical teams to develop improved lead candidates and file 3 FDA INDs.

Postdoctoral Research Fellow

Yale University School of Medicine

08/1999 - 08/2001 New Haven, United States

- Conducted cloning, expression, purification, and crystallographic analysis of the cytoplasmic region of Erythropoietin Receptor and JAK protein kinase.

EDUCATION

D Phil (PhD)

University of Oxford, Laboratory of Molecular Biophysics

08/1995 - 08/1999 Oxford, United Kingdom

- Structural Studies of Cytokines and Cytokine Receptors.

B.Sc.

University of Leeds, Biochemistry and Molecular Biology

08/1991 - 08/1995 Leeds, United Kingdom

- First Class Honors, US equivalent: A or 70-100%.

PATENTS

Anti-mutant Calreticulin (CALR) Antibodies and uses thereof, 2022

https://patents.google.com/patent/WO2023107994A1/en

Bicyclic Compounds as Inhibitors of WRN

Pending

CONTINUED LEARNING

2025 - Google: Foundations of Project Management

https://www.coursera.org/account/accomplishments/verify/605BGOEB1YGC

2025 - IBM: Introduction to Artificial Intelligence

https://www.coursera.org/account/accomplishments/verify/71R8R1FHA194

2025 - AWS: Serverless Architectures

https://www.coursera.org/account/accomplishments/verify/X9AD2JWH2HE9

2024 - Google: Foundations: Data, Data, Everywhere

https://www.coursera.org/account/accomplishments/verify/4S09Q8ICKGXN

WEB AND NEWS

Blog

https://marcdeller.com

www.linkedin.com/in/marccdeller

marccdeller

My Google Scholar

https://bit.ly/marcdeller_pubs

My Protein Structures

https://bit.ly/marcdeller_proteins

Mentored Lemelson-MIT Student Prize

https://news.stanford.edu/stories/2017/04/undergrads-win-prize-work-combating-antibacterial-resistance

Your one-stop shop for producing, crystallizing biomolecules

https://med.stanford.edu/news/all-news/2016/04/your-one-stop-shop-for-producing-crystallizing-biomolecules.html

Top articles in structural biology (Spring 2020)

https://journals.iucr.org/special_issues/2020/biologytoparticles/index.html

SKILLS

General Science and Personal

Molecular Sciences, Protein Structure Determination, Platform Optimization, X-ray Crystallography, Cryo-EM, Protein Expression (bacterial, mammalian, insect, cell-free), Protein Purification, Construct Design, Protein Engineering, Biophysical Characterization (SPR/BLI/DSF/ITC/DLS/Massphotometry), Lab Automation, Membrane Proteins, Hit-to-Lead, AI/ML, Cloud Computing, Validation of Protein Co-Complexes, Computational Chemistry, Structure-Based Drug Discovery, Fragment-Based Drug Discovery, Accelerated Data Strategy, Project Management, Strategic Thinking, Cross-Functional Collaboration, Effective Communication, External CRO Capabilities.

COMPUTATIONAL SKILLS

Protein Structure

HKL2000/3000, CCP4, PHENIX, PyMOL, COOT, Schrödinger, CCG/MOE, GROMACS, ALPHAFOLD, RFDiffusion, ProteinMPNN, RELION, CryoSPARC, R/Shiny, Python, RDKit/PANDAS, ChemCart, LLAMA, PERPLEXITY, ChatGTP, Globus, AWS, Spotfire, SLURM, ELN/LIMS, PSILO.

Data Analysis and AI

R/Shiny, Spotfire, GraphPad/Prism, MATLAB, Python, RDKit/PANDAS, ChemCart, Nanome, LLAMA, PERPLEXITY, ChatGTP, Word, PowerPoint, Access, Excel, Canva, Adobe, JIRA, Confluence, Smartsheets, LIMS, ELN, Globus, AWS

CONTINUED LEARNING

2024 - Coursera: Introduction to R: Basic R syntax
https://www.coursera.org/account/accomplishments/verify/T687VG5UYI5O

2024 - Coursera: Dashboard Development with Shiny: GenAI for Retail Analysis
https://www.coursera.org/account/accomplishments/verify/OO09W4LMZGCB

2024 - Linkedin: Amplify Your Communication Skills with Generative AI
https://www.linkedin.com/learning/certificates/e73941e7b279574ef2e43e461acd40efb644f9284f285d1210cee7580ee9528a

REFERENCES

Dr. Adam Lee, Head of Data Logistics, Incyte
alee@incyte.com

Dr. Guofeng Zhang, Head of Biochemistry and Structural Biology, Incyte
guzhang@incyte.com

LATEST PUBLICATIONS (60 TOTAL)

https://bit.ly/marcdeller_pubs

Full list at Google Scholar
https://bit.ly/marcdeller_pubs

Discovery of INCB159020, an Orally Bioavailable KRAS G12D Inhibitor

J. Med. Chem.

Qinda et al.

2025 https://pubs.acs.org/doi/abs/10.1021/acs.jmedchem.4c02662

Support for KRAS IND filing: Discovered an innovative, orally bioavailable inhibitor for the KRAS G12D mutation, which is known for its role in driving cancer. The objective is to effectively balance potency and ADME properties in order to tackle the challenges associated with this previously "undruggable" protein. This development aims to broaden treatment options beyond therapies specifically targeting the KRAS G12C mutation in lung cancers.

Discovery of (4-pyrazolyl)-2-aminopyrimidines as potent and selective Inhibitors of cyclin-dependent kinase 2

J. Med. Chem.

JR Hummel et al.

2024 https://pubs.acs.org/doi/abs/10.1021/acs.jmedchem.3c02287

Support for CDK2 IND filing: Protein structure-based design of a first-in-class potent and highly selective CDK2 inhibitor from a novel chemical class, which demonstrates antitumor activity and addresses historical limitations of toxicity and poor selectivity that hindered the development of previous CDK2-targeted cancer therapies.

Discovery of potent and selective inhibitors of wild-type and gatekeeper mutant fibroblast growth factor receptor (FGFR) 2/3

J. Med. Chem.

Artem Shvartsbart et al.

2022 https://pubs.acs.org/doi/abs/10.1021/acs.jmedchem.2c01366

Support for FGFR2/3 IND filing: Details the discovery of novel, selective FGFR2/3 inhibitors that address critical limitations of existing cancer treatments by maintaining efficacy against drug-resistant mutations and reducing side effects like hyperphosphatemia, thereby offering a promising therapeutic advancement for patients with cancers such as cholangiocarcinoma and bladder cancer

MOST CITED PUBLICATIONS

Crystal structure of a soluble cleaved HIV-1 envelope trimer

Science, 979 citations

JP Julien, A Cupo, D Sok, RL Stanfield, D Lyumkis, MC Deller et al.

2013 https://www.science.org/doi/abs/10.1126/science.1245625

Exciting paper: Presents a high-resolution crystal structure of a near-native, cleaved HIV-1 envelope trimer in complex with a broadly neutralizing antibody, revealing unprecedented molecular details of the trimer's architecture and its vulnerable sites—insights that are crucial for both understanding how HIV-1 infects cells and advancing rational vaccine design

Supersite of immune vulnerability on the glycosylated face of HIV-1 envelope glycoprotein gp120

Nature structural & molecular biology, 420 citations

Leopold Kong et al.

2013 https://www.nature.com/articles/nsmb.2594

This study reveals: How the HIV-1 glycan shield's Asn332-dependent supersite—a densely glycosylated region on gp120—can be penetrated by diverse antibodies like PGT 135, which uses elongated CDR loops to bypass glycans and target vulnerable protein surfaces, offering a blueprint for designing vaccines that exploit this Achilles' heel of the virus

Protein stability: a crystallographer's perspective

Structural Biology and Crystallization Communications, 370 citations

Marc C Deller, Leopold Kong, Bernhard Rupp

2016 https://journals.iucr.org/f/issues/2016/02/00/en5571/index.html

Featured as a "Top article in structural biology (Spring 2020)": Details practical, crystallographer-focused discussion on protein stability, the understanding of which is essential for optimizing critical processes like protein expression, purification, formulation, storage, and structural studies across the biotechnology, pharmaceutical, and academic sectors.

The Role of the Secondary Coordination Sphere in a Fungal Polysaccharide Monooxygenase

ACS chemical biology, 130 citations

Elise A Span, Daniel LM Suess, Marc C Deller, R David Britt, Michael A Marletta

2017 https://pubs.acs.org/doi/abs/10.1021/acschembio.7b00016

This study elucidates: Critical hydrogen-bonding networks in fungal polysaccharide monooxygenases (PMOs) that govern oxygen activation and proton transfer—key mechanistic insights for optimizing enzymatic cellulose degradation, with transformative potential for biofuel production and sustainable biomass utilization.

LATEST PUBLICATIONS (60 TOTAL)

Structure–function analysis of the extended conformation of a polyketide synthase module

Journal of the American Chemical Society

Xiuyuan Li, et al.

2018 https://pubs.acs.org/doi/abs/10.1021/jacs.8b02100

Groundbreaking study: Resolves a long-standing debate in polyketide synthase (PKS) biology by demonstrating—via innovative antibody stabilization, structural validation (X-ray/SAXS), and kinetic assays—that the extended module conformation is catalytically functional for both chain elongation and modification, unlocking critical insights for engineered antibiotic production.

Validation of Protein–Ligand Crystal Structure Models: Small Molecule and Peptide Ligands

Protein Crystallography: Methods and Protocols

Edwin Pozharski, Marc C Deller, Bernhard Rupp

2017 https://link.springer.com/protocol/10.1007/978-1-4939-7000-1_25

Emphasizes need for high-quality protein structures in the age of predictive AI: Highlights the critical need for robust validation of protein-ligand structural models, which are essential for drug discovery, by outlining specific criteria like electron density fit, stereochemistry, and binding plausibility, and introducing tools to assist researchers in this often challenging validation process due to scarce experimental data for ligands.

Lipid interactions and angle of approach to the HIV-1 viral membrane of broadly neutralizing antibody 10E8: Insights for vaccine and therapeutic design

PLoS pathogens

Adriana Irimia et al.

2017

https://journals.plos.org/plospathogens/article?id=10.1371/journal.ppat.1006212

Landmark study: Redefines HIV-1 neutralization by revealing—via X-ray structures, mutagenesis, and modeling—that the broadly protective 10E8 antibody targets a hybrid epitope combining the gp41 MPER region and viral membrane lipids, with its light chain engaging lipids and positioning MPER perpendicularly to the membrane, offering transformative insights for designing lipid-informed vaccines/therapeutics against HIV.

Key gp120 glycans pose roadblocks to the rapid development of VRC01-class antibodies in an HIV-1-infected Chinese donor

Immunity

Leopold Kong et al.

2016 https://www.cell.com/immunity/fulltext/S1074-7613(16)30095-4

Pivotal study: Bridges critical gaps in HIV vaccine design by uncovering—through structural analyses (X-ray/EM), longitudinal tracking, and functional assays—how early VRC01-class antibody precursors overcome glycan obstacles via light-chain adaptations, revealing both roadblocks (N276/V5 glycan clashes) and a rapid maturation pathway for broad neutralization, guiding next-gen immunogens targeting the CD4-binding site.

Complete epitopes for vaccine design derived from a crystal structure of the broadly neutralizing antibodies PGT128 and 8ANC195 in complex with an HIV-1 Env trimer

Biological Crystallography

Leopold Kong et al.

2015 https://journals.iucr.org/paper?S1399004715013917

Structural tour de force: Illuminates HIV-1's glycan shield dynamics by resolving—via high-resolution crystallography of the BG505 SOSIP trimer with 8ANC195/PGT128—how bNAbs exploit gp41 interactions (N637 glycan accommodation) and glycan domino effects (N301 repositioning N262), unveiling allosteric glycan manipulation and completing trimer-level epitope blueprints for precision vaccine engineering.

MOST CITED PUBLICATIONS

Models of protein–ligand crystal structures: trust, but verify

Journal of computer-aided molecular design, 113 citations

Marc C Deller, Bernhard Rupp

2015

https://link.springer.com/article/10.1007/s10822-015-9833-8

This paper is crucial: Establishes metrics underscoring why X-ray crystallography is the gold standard for creating precise protein-ligand models—essential for advancing drug design and computational biology—while advocating rigorous validation to combat overinterpretation and ensure reliability in scientific research.

PUBLICATIONS (MISC)

2017

- Crystallisation of Proteins and Macromolecular Complexes: Past, Present and Future
  MC Deller, B Rupp
  eLS

2015

- Crystal structure of a two-subunit TrkA octameric gating ring assembly
  MC Deller, HA Johnson, MD Miller, G Spraggon, MA Elsliger, IA Wilson, ...
  Plos one 10 (3), e0122512

2014

- Approaches to automated protein crystal harvesting
  MC Deller, B Rupp
  Structural Biology and Crystallization Communications 70 (2), 133-155

2012

- Structure of hepatitis C virus envelope glycoprotein E2 antigenic site 412 to 423 in complex with antibody AP33
  L Kong, E Giang, T Nieusma, JB Robbins, MC Deller, RL Stanfield, ...
  Journal of virology 86 (23), 13085-13088

2012

- Functional and structural characterization of a thermostable acetyl esterase from *Thermotoga maritima*
  M Levisson, GW Han, MC Deller, Q Xu, P Biely, S Hendriks, LF Ten Eyck, ...
  Proteins: Structure, Function, and Bioinformatics 80 (6), 1545-1559

2000

- Crystal structure and functional dissection of the cytostatic cytokine oncostatin M
  MC Deller, KR Hudson, S Ikemizu, J Bravo, EY Jones, JK Heath
  Structure 8 (8), 863-874

2000

- Cell surface receptors
  MC Deller, EY Jones
  Current opinion in structural biology 10 (2), 213-219