Extended Portfolio - Marc C. Deller, D Phil

Structural Biology | Drug Discovery | X-ray Crystallography | Cryo-EM

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PATENTS

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

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

Bicyclic Compounds as Inhibitors of WRN, pending

LATEST PUBLICATIONS (60 TOTAL)

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

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.

WEB AND NEWS

Blog

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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

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

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

LATEST PUBLICATIONS (60 TOTAL)

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.

PUBLICATIONS (CONT)

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

2015

- Structure-based discovery of NANOG variant with enhanced properties to promote self-renewal and reprogramming of pluripotent stem cells
  Y Hayashi, L Caboni, D Das, F Yumoto, T Clayton, MC Deller, P Nguyen, ...
  Proceedings of the National Academy of Sciences 112 (15), 4666-4671

2014

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

2014

- Structural insights into the recognition of phosphopeptide by the FHA domain of kanadaptin
  Q Xu, MC Deller, TK Nielsen, JC Grant, SA Lesley, MA Elsliger, ...
  PLoS One 9 (9), e107309

2012

- Crystal Structure of the First Eubacterial Mre11 Nuclease Novel Features that May Discriminate Substrates During DNA Repair
  D Das, D Moiani, HL Axelrod, MD Miller, D McMullan, KK Jin, P Abdubek, ...
  J. Mol. Biol 397: 647

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

2010

- Structure of the γ-D-glutamyl-L-diamino acid endopeptidase YkfC from Bacillus cereus in complex with L-Ala-γ-D-Glu: insights into substrate recognition by NlpC/P60 cysteine ...
  Q Xu, P Abdubek, T Astakhova, HL Axelrod, C Bakolitsa, X Cai, D Carlton, ...
  Structural Biology and Crystallization Communications 66 (10), 1354-1364

PUBLICATIONS (MOST CITED, 3631 TOTAL)

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.

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 (CONT)

📅 2010

- The crystal structure of a bacterial Sufu-like protein defines a novel group of bacterial proteins that are similar to the N-terminal domain of human Sufu
  D Das, RD Finn, P Abdubek, T Astakhova, HL Axelrod, C Bakolitsa, X Cai, …
  Protein science 19 (11), 2131-2140

📅 2010

- Bacterial pleckstrin homology domains: a prokaryotic origin for the PH domain
  Q Xu, A Bateman, RD Finn, P Abdubek, T Astakhova, HL Axelrod, …
  Journal of molecular biology 396 (1), 31-46

📅 2009

- Structural basis of murein peptide specificity of a γ-D-glutamyl-L-diamino acid endopeptidase
  Q Xu, S Sudek, D McMullan, MD Miller, B Geierstanger, DH Jones, …
  Structure 17 (2), 303-313

📅 2009

- A structural basis for the regulatory inactivation of DnaA
  Q Xu, D McMullan, P Abdubek, T Astakhova, D Carlton, C Chen, HJ Chiu, …
  Journal of molecular biology 385 (2), 368-380

📅 2008

- Crystal structures of MW1337R and lin2004: Representatives of a novel protein family that adopt a four-helical bundle fold
  P Kozbial, Q Xu, HJ Chiu, D McMullan, SS Krishna, MD Miller, P Abdubek, …
  Proteins: Structure, Function, and Bioinformatics 71 (3), 1589-1596

📅 2007

- Crystal structures of two novel dye-decolorizing peroxidases reveal a β-barrel fold with a conserved heme-binding motif
  C Zubieta, SS Krishna, M Kapoor, P Kozbial, D McMullan, HL Axelrod, …
  Proteins: Structure, Function, and Bioinformatics 69 (2), 223-233

📅 2007

- Identification and structural characterization of heme binding in a novel dye-decolorizing peroxidase, TyrA
  C Zubieta, R Joseph, S Sri Krishna, D McMullan, M Kapoor, HL Axelrod, …
  Proteins: Structure, Function, and Bioinformatics 69 (2), 234-243

📅 2000

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

📅 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