DEPARTMENT OF
# Biochemistry & Molecular Biology

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**Special Seminar**

## Dr. Kale Kundert

Harvard Medical School

**Wednesday, May 7th, 2025**

11:00 a.m. – on Zoom

https://msu.zoom.us/j/92837548243
Meeting ID: 928 3754 8243

# "Deep learning for designing protein/non-protein ligand interactions"

Intrinsically disordered domains represent a challenging frontier in protein structure. I will discuss a new computational method to remodel protein backbones in regions lacking regular secondary structure, a key step in the ability to rationally design functional proteins. One application for modeling novel protein/non-protein interactions relates to synthetic biology, specifically through the design of novel amino acyl tRNA synthetases, i.e. the enzymes responsible for charging tRNAs with their cognate amino acids.


Krivacic C, **Kundert K,** Pan X, Pache RA, Liu L, Ó Conchúir S, Jeliazkov JR, Gray JJ, Thompson MC, Fraser JS, Kortemme T. Accurate positioning of functional residues with robotics-inspired computational protein design. Proc. Natl. Acad. Sci. U.S.A. 119:11:e2115480119 (2022).

**Kundert K**. Wellmap: A file format for microplate layouts BMC Res. Notes. 14:164 (2021).

**Kundert K**, Lucas JE, Watters KE, Fellmann C, Ng AH, Heineike BM, Fitzsimmons CM, Oakes BL, Savage DF, El-Samad H, Doudna JA, Kortemme T. Controlling CRISPR-Cas9 with ligand-activated and ligand-deactivated sgRNAs. Nat. Commun. 10:2127 (2019).

**Kundert K**, Kortemme T. Computational design of structured loops for new protein functions. Biol. Chem. 400:3:275–288 (2019).