

## **Seminar 2017**

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### **Protein structure determination using metagenome sequence data**



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Despite decades of work by structural biologists, there are still ~5200 protein families with unknown structure outside the range of comparative modeling. We show that Rosetta structure prediction guided by residue-residue contacts inferred from evolutionary information can accurately model proteins that belong to large families and that metagenome sequence data more than triple the number of protein families with sufficient sequences for accurate modeling. We then integrate metagenome data, contact-based structure matching, and Rosetta structure calculations to generate models for 614 protein families with currently unknown structures; 206 are membrane proteins and 137 have folds not represented in the Protein Data Bank. This approach provides the representative models for large protein families originally envisioned as the goal of the Protein Structure Initiative at a fraction of the cost.

**Laufer Center Conference Room**  
**Thursday, November 30th**  
**11:00 am - 12pm**  
**Host: Dill Group**

For a disability related accommodation,  
please call 631-632-5400