Medical Informatics Group

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Gil Alterovitz's lab

Harvard Medical School

- **Presenter:** Ashay Athalye

- **Title:** Machine learning characterization and prediction of intrinsically disordered protein interactions: A focus on BRCA1

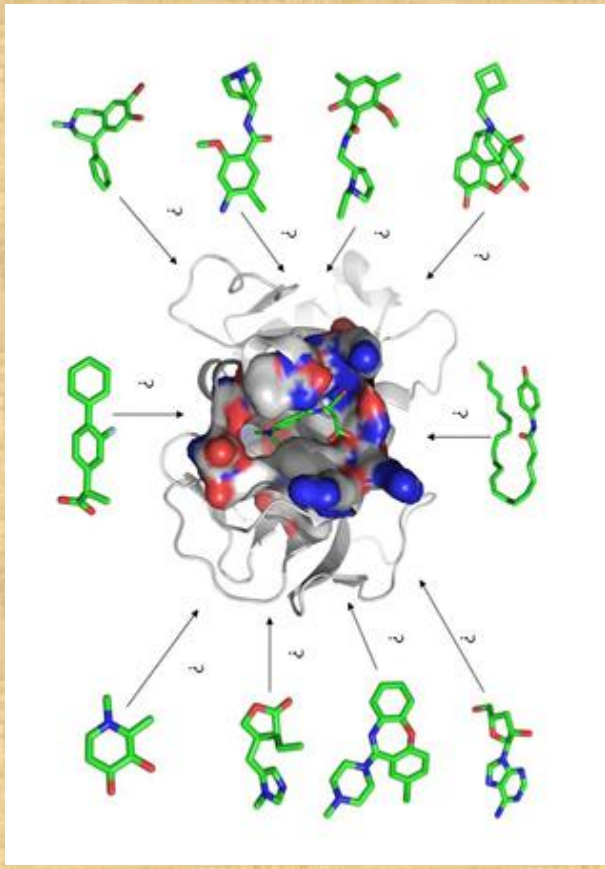
- **Result:** BRCA1 protein functions both individually as well as jointly in protein complexes, and that proteins that form functional complexes with BRCA1 also have separate independent functions

- **Presenter:** Arul Prasad

- **Title:** The Significance of Disordered Residues in: 1) Bacterial Drug Resistance and 2) SNP Interactions in relation to Disease Associations

- **Result:** found significant residue ranges in bacterial drug resistance and significant categories of SNPs in protein interactions that have disease association

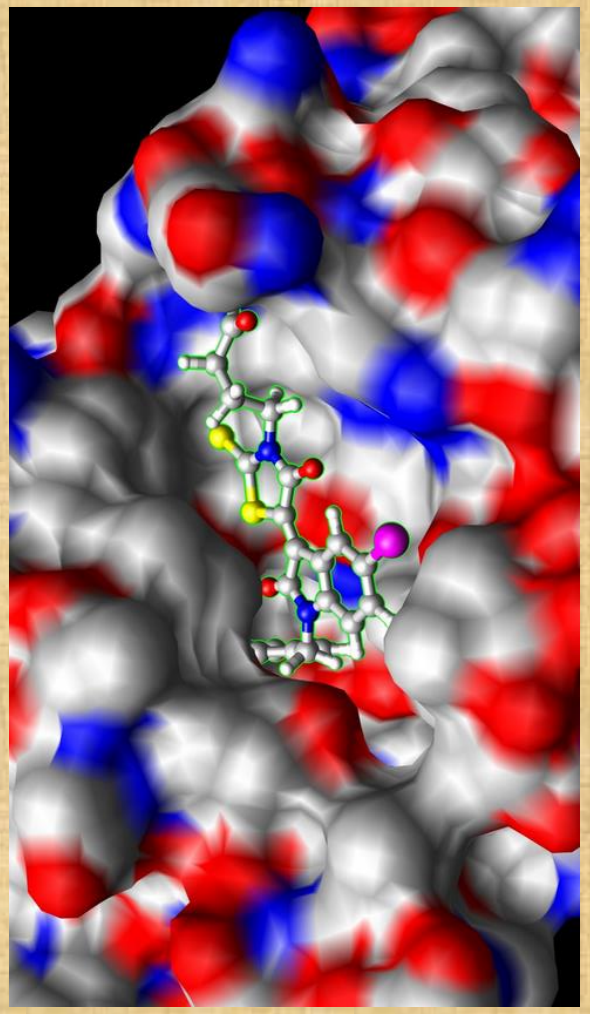
- **Presenter:** Kara Luo
- **Title:** Computer Simulation of Biosynthetic Modifications to Improve Binding Activity
- **Result:** improvements for existing drug molecules that target the disordered protein region of Enterococcus Faecium



- **Presenter:** Andrew Li

- **Title:** Exploring Multi-conformational Modeling and Flexibility of Molecular Recognition Features In Improving Drug Docking

- **Result:** demonstration of how flexibility based modeling of an IDP improves IDP-drug conventional docking and the investigation of a novel paradigm for docking to reduce runtime



- **Presenter:** Daniel Lu
- **Title:** Investigating drug synergy mechanisms of disordered protein-related diseases
- **Result:** found pairs of drugs that would likely achieve drug synergy for Human Papillomavirus and several other diseases