Van der Waals packing facilitates membrane protein association

Abstract

Visual Abstract

Design algorithm, experiment, fluorescence correlation

Introduction

Describe in detail how other studies use a combination of assays like TOXGREEN (term?) to study membrane proteins and why they’re difficult

Why combine computational design to probe this: high-throughput, can’t solve structures of that many but reference papers and information of structures

WHY ARE WE USING MSL…: maybe I’ll let Alessandro write/beef this part up, if he even feels the need to mention it in detail

Mention a paragraph specifically for membrane protein dimers significance

Results

* 4-5 figures (maybe one table?)

Figure 1A: Modeling the membrane protein dimer geometric space

1B: Design of Membrane protein dimers (similar to how some of the coding papers do it?)

* Add detail here (names: DEE, IMM1, SCWRL4, MSL, etc.)

Figure 2A: Fluorescence Reconstruction general data (distribution of all proteins fluorescence)

2B: more general data about fluorescence; maybe separate into different graphs (what other types of graphs can I use to represent fluorescence? Bar graphs with number of designs from each region that made it through; could also have bar graphs for their expected geometries here

2C: Another schematic about their geometries here?

Figure 3A: Energy score vs fluorescence

3B: separate energy scores vs fluorescence here

3C: if we do regression analysis, could add that here

3D: also can add in geometry data for this set of structures; just the parsed data from clashing mutants

3E: void mutant data, also potentially from void mutants

Figure 4A: Conversion to deltaG

4B: snippets of westerns? Or at least quantification from westerns? Maltose test in supplement?

Discussion

Van der waals facilitates…x amount…approximately x% of GASright, known for Hbonding. Can we conclude anything about the contribution of van der Waals in GASrights and other regions of proteins? Are there any other studies that have left/right handed structures that do experiments that demonstrate packing/dimerization ability? Or portions of proteins found in some of these structures (maybe coiled-coil FtsLB data? What conclusions if any can be drawn from these? If they exist, could I take a look at the distribution of known proteins and their sequences/interfacial residues (any way to do this computationally?) and compare to them? I could at the very least compare to the residues found in the structures that I extracted from and see if this gives me any insight? Would it be possible to look at them positionally? Or at least look at the most similar structures by RMSD or something?

Methods

* Many supplementary figures
  + More details in the starter outline