Whitefish Bay High School SMART Team

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The Ricin Fall of Select Agents

PDB: 2AAI


Format: Alpha carbon backbone

RP: Zcorp with plaster

Description:
Ricin has a long history of use as a weapon of terrorism. Ricin attacks have been planned and thwarted by terrorist groups in the United States and across the globe. Ricin, generated from castor beans, is fatal to humans because it causes cell death. Ricin is a protein composed of two chains, A and B, linked by a disulfide bond. The A chain detaches from the B chain, and in the active site, Glu177 de-adenylates a base on RNA found within the 60S ribosome, thus inhibiting cellular protein synthesis. The A chain is composed of three domains: one characterized by a five-stranded beta sheet, one by five alpha helices, and the final by a disc-like shape. The B chain facilitates entry into the cell by binding to surface receptors. The B chain is composed of two nearly identically-folded domains that share high amino acid similarity. The ligands are Gal264, whose domain is defined by Asn46, Lys40, and Asp22, and Gal267, whose domain is defined by Asn255 and Asp234. The Whitefish Bay High School SMART Team (Students Modeling A Research Topic) modeled ricin using 3D printing technology to better understand its function and structure. Further research is required to develop a vaccine, although two putative formulations exist: RiVax and RiVEc. Unexpectedly, these vaccines are composed of the A chain, rather than the receptor binding B chain. A successful vaccine could be given primarily to military and national security personnel to prevent the deadly effects of biological military action using ricin.

Specific Model Information:

Amino acid side chains involved:
- Glu177 - darksalmon: part of active site of the deadenylation of the 60s ribosome
- Gal264 and Gal267 - blue: ligands around which the B chain forms its two nearly identical domains
- Asn46 and Lys40 - red: form hydrogen bonds to the Gal264 ligand and determine epimeric specificity
- Asp22 - purple: forms hydrogen bond to Asn46 and holds it in place
- Asn255 - gold: forms hydrogen bonds to the Gal267 ligand and determines epimeric specificity
- Asp 234 - chocolate: forms hydrogen bond to Asn255 and holds it in place

Highlighted protein structures:
- Alpha helix structures are colored chartreuse
- Beta sheet structures are colored fuchsia
- Hydrogen bonds are colored palegoldenrod
- A chain backbone is colored white
- B chain backbone is colored lightblue
- Disulfide bonds are colored yellow
  - The two amino acids that form the disulfide bond that connects the two domains are also colored yellow, solely for the purpose of emphasizing that bond

Supporting Features:
- Struts are colored gray

CBM SMART Teams Website:
http://cbm.msoe.edu/smartTeams/smartTeamsLocal.php