

## Bioinf 301 Assignment #6 – Structure Prediction & Modeling

Nov. 24, 2011

A protein has recently been isolated from a small nanobacterium called *Nanocoli reductis*. This particular strain of nanobacteria has been found to be quite useful in the conversion of CO<sub>2</sub> to methane. This type of reaction could be quite important for the development of a novel carbon capture technology. The protein that seems to facilitate this reaction has been isolated and it has the following sequence:

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      10      20      30      40      50      60
MTDRLVHISN NSYGTNIMRG DAGMLINYWG QWCAPCRLMA PLIEDVADQF EGRMCVARAD

      70      80      90      100
INEDPGTAKP FGLKGIPTVI LYRNGEILAS KVAAATKANL REWMEAKLG
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- 1) Using the above information, predict the secondary structure of this protein. Describe which method(s) you used and why (max ½ page).
- 2) Using the above information, predict the 3D structure of this protein. Describe which method(s) or server(s) you used. From the predicted coordinates generate a high quality, **colour** image of the predicted structure (max 1 page). Do not staple any PDB coordinate data to your answer sheet.
- 3) Assess the quality of the structure you have generated. Use graphs or tables to illustrate your points about the structure's quality. **Do not** provide pages of uninterpreted web server output. You must provide a synopsis and a written interpretation to receive any grade for this question (max 2 pages).
- 4) What is the distance (in Angstroms) between:
  - a) the CA atom of residue 42 and the CB atom of residue 45?
  - b) the N atom of residue 1 and the C atom of residue 109?
- 5) What are the phi/psi torsion angles for residues 80-90?
- 6) Compare the structure of this protein to all other structures in the PDB. Which structure is most similar to this protein? (max 1 page)
- 7) What is the possible name and/or function of this protein?

**Assignment due on Dec. 1, 2011 by 11:00 am (10% off for each day late)**