

LEK_9_Structure

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1 Structural Bioinformatics

1.1 Protein Structures

Name three structural planes of protein structures.

1. Primary structure (amino acid sequence)
2. Secondary structure (α -helix, β -sheet, turn)
3. Tertiary structure (three-dimensional structure formed by assembly of secondary structure)

1.2 PyMol

Give an example for the syntax in PyMol for creating the three selections below:

1. Select Chain A of your structure.

```
select ChA, chain A
```

2. Select all Amino Acids in Helices in your structure.

```
select Helices, ss h
```

3. Select all prolines in your structure

```
select PRO, resn Pro
```

1.3 Modelling

Name the three methods you could use to generate protein structure models in silico.

1. Homology or comparative modelling
2. Threading (fold recognition) modelling
3. *Ab initio* (*de novo*, new folds) modelling (*ab initio*: “from the beginning”)