Practical 11

Questions

4 April 2022

1. Find the propensity of alpha helices using the following sequence and secondary structure assignments.

```
Sequence: LGASGIAAFAFGSTAILIILFNMAAEVHFDPLQFFRQFFWLGLYPPKAQY
Sec. str: XHHHHHHHHHHHHHHHHHHHHHHHHHXXXXXXXXXXXXXXXXXXXXXXX

Sequence: GMGIPPLHDGGWWLMAGLFMTLSLGSWWIRVYSRARALGLGTHIAWNFAA
Sec. str: XXXXXXXXXXHHHHHHHHHHHHHHHHHHHHHHHHHHHHHXHHHHHHHHH

Sequence: AIFFVLCIGCIHPTLVGSWSEGVPFGIWPHIDWLTAFSIRYGNFYYCPWH
Sec. str: HHHHHHHHHXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXHHH

Sequence: GFSIGFAYGCGLLFAAHGATILAVARFGGDREIEQITDRGTAVERAALFW
Sec. str: HHHHHHHHHHHHHHHHHHHHHHHXXXXXXXXXXXXXXXXXXXXXXXXX
```

2. Find the propensity of alpha helices manually for the sequence in question 1.

3. Using the rules for helices and strands, identify the helical and strand segments in the following sequence

```
KVFGRCELAAAMKRHGLDNYRGYSLGNWVCAAKFESNFNTQATNRNTDGSTDYGILQINSRWWCNDGRTPGSRNLCNI
PCSALLSSDITASVNCAKKIVSDGNGMNAWVAWRNRCKGTDVQAWIRGCRL
```

Hint: **Helix**: Assign 1 for H_α and h_α; 0.5 for I_α; 0 for i_α; -1 for B_α and b_α; identify 6-residue segments with score more than or equal to 4; extend it until the actual value (Table 5.2) for last four residues is less than 4. Continue the search.

Strand:

Assign 1 for H_β and h_β; 0.5 for I_β; 0 for i_β; -1 for B_β and b_β; identify 5-residue segments with score more than or equal to 3; extend it until the actual value for the last three residues is less than 3.

For conflicting situation: compare the values and assign the secondary structure based on the highest value

TABLE 5.2 Chou–Fasman parameters

Residue	P_α	Residue	P_β
Glu	H_α 1.53	H_β Met	1.67
Ala	1.45	Val	1.65
Leu	1.34	Ile	1.60
His	h_α 1.24	h_β Cys	1.30
Met	1.20	Tyr	1.29
Gln	1.17	Phe	1.28
Trp	1.14	Gln	1.23
Val	1.14	Leu	1.22
Phe	1.12	Thr	1.20
Lys	I_α 1.07	Trp	1.19
Ile	1.00	I_β Ala	0.97
Asp	i_α 0.98	i_β Arg	0.90
Thr	0.82	Gly	0.81
Ser	0.79	Asp	0.80
Arg	0.79	b_β Lys	0.74
Cys	0.77	Ser	0.72
Asn	b_α 0.73	His	0.71
Tyr	0.61	Asn	0.65
Pro	B_α 0.59	Pro	0.62
Gly	0.53	B_β Glu	0.26

4. Verify one of the helical and strand segments, manually.

Deadline: 10 April 2022