**Predoc course 2019 - Structural week**

**Computational practical - Gibson team**

Duration: 3.5 hours

**Guidelines and Suggestions**

-Keep talks short

-Ask questions and interact at the beginning and middle of talk

-Consider group activities for the practical part

-Don’t use too much text in slides, put main message of the slide as title

-Add more articles or links to these lists so we can prepare a handout

**Part 1**

Talk (20 min)

* Bioinformatics in protein Science
* Sequence-Structure relation
* Structure and Disorder
* Signaling and PPI (Hubs, PTM)

Practical (20-30 min)

* Uniprot
* String, PhosphoDB
* ClustalO, Jalview
* PDB, Disprot, IUPRED (X-ray, NMR)
* Homology modelling

References:

[a] Forman-Kay, J. D. & Mittag, T. (2013) “From Sequence and Forces to Structure, Function, and Evolution of Intrinsically Disordered Proteins.” *Structure*. 21(9):1492-1499. ([Article](https://www.sciencedirect.com/science/article/pii/S096921261300292X)).

**Part 2**

Talk (20 min)

* SLiMs
* Computational approaches
* High-throughput experimental approaches

Practical (20-30 min)

* ELM (Find motifs in alignments [order-disorder protein], REGEX)
* Chimera (Superposition, Different types of bonding)
* Motif high-throughput data

References:

[a] Tompa, P et al. (2014) “A million peptide motifs for the molecular biologist.” *Molecular cell review*. 55:161-169. ([Article](https://www.sciencedirect.com/science/article/pii/S1097276514005620)).

[b] Gibson, T et al. (2015) “Experimental detection of short regulatory motifs in eukaryotic proteins: tips for good practice as well as for bad.” *Cell Commun Signal*. 13:42. ([PDF](https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4652402/pdf/12964_2015_Article_121.pdf)).

[c] Davey, N. E. et al. (2012) “Attribute of short linear motifs.” *Mol. BioSyst*. 8:268-281. ([PDF](https://pubs.rsc.org/en/content/articlepdf/2012/mb/c1mb05231d)).

[d] Ivarsson, Y & Jemth, P. (2019) “Affinity and specificity of motif-based protein–protein interactions.” *Current Opinion in Structural Biology*. 54:26-33. ([Article](https://www.sciencedirect.com/science/article/pii/S0959440X18301155)).

–20 min break–

**Part 3**

Talk (20 min)

* Integrative approaches for motif discovery
* Motifs in viral and bacterial infections

Practical (20-30 min)

* Finding motifs through ELM
* Motif prediction in pathogens

References:

[a] Davey, N et al. (2011) “How viruses hijack cell regulation.” *Trends in Biochemical Sciences*. 36(3):159-169. ([Article](https://www.sciencedirect.com/science/article/pii/S0968000410002008)).

**Part 4 – Presentation materials**

(30 min)