Protein Interactions: Computational Techniques

Assignment - 2

Corse: BT6320 **Marks: 20**

Questions

• Use the same drugs you selected in QSAR (previous) assignment

• Perform Pharmacophore modelling (BIOVIA software) with 5 drugs so that you get a good overlap

• Identify 30 new structures from Zinc15 that have this pharmacophore (ZINCPHARMER software)

• Test drug likeness properties/ADME (SWISS ADME/PkCSM)

• Select 20 best candidates

• Dock all these with the target (if target pdb is not available do a homology modelling)

• Dock the original 10 drugs you selected from literature also to the same target

• Compare the results in a table form

• Prepare a report with introduction /methodology / .Results /discussions/Conclusion

Last date for submission 30 Oct 2024