Hi Jeremy,

As promised, here are my two questions for your prelim exam:

1) QSAR models typically rely on 2D and 3D molecular descriptors to characterize small molecules. However, those molecules are highly flexible and those conformation-dependent parameters are not taken into account in the vast majority of QSAR modeling studies. Introduce and review the concept of 4D-QSAR across literature studies (based on series of conformations and/or MD trajectories). Describe the challenges and potential benefits of using such conformation-dependent modeling technique.

2) Cheminformatics techniques have been developed to characterize and model kinase-inhibitor interactions. However, little is known about the potential use of these techniques for differentiating highly similar kinases and better understanding the apparent selectivity of certain small molecule ligands towards one particular kinase. Define and discuss these concepts using the example of the two kinases ERK1 and ERK2. Give preliminary modeling results if possible.