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Proteins in harmony: Tuning selectivity in early drug discovery

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Propositions

Proteins in Harmony Tuning Selectivity in Early Drug Discovery

1. Drug target identification is one of the most important, but also most complex, aspects of preclinical drug development. In this respect, computational target prediction is a highly valuable tool to identify the most probable targets for a compound under investigation.

This thesis, chapter 2

2. Computational target prediction methods rely on the general assumption that similar molecules will have similar interactions.

This thesis, chapter 2

3. The intrinsic variety in chemical structure of active compounds implies that there may be multiple binding sites.

This thesis, chapter 3

4. One cannot simply model selectivity without taking context into consideration.

This thesis

5. Better quality data mean more and higher confidence assertions and therefore more robust applications and models.

G. Papadatos et al. J Comput Aided Mol Des. 2015; 29:885–896.

6. Molecules with optimal multitarget activities have the potential of improving efficacy and safety of drugs in the therapy of complex diseases.

A. Anighoro et al. J Med Chem 2014; 57:7874–7887.

7. Commonly used ‘random split’ partitioning might lead to an overly optimistic performance estimate.

E.B. Lenselink et al. J Cheminform. 2017; 9:45.

8. All researchers, including medicinal chemists, will have to become comfortable working in data-rich environments.

S.J. Lusher et al. Drug Discov Today. 2014; 19: 859–868.

9. Time spent on teaching is time lost on research, but not on science.

10. Why spend energy on breaking the glass ceiling? Just build a house without any.

11. Float like a butterfly, sting like reviewer nr 3.

Adapted from Muhammad Ali

12. “You can Google that” is the worst advice when translating bash’s concatenate into python: “cat in python”.