



Prague, 23. 3. 2023

## Review of the doctoral thesis “Prediction of ligand binding sites from protein structure” by Mgr. Radoslav Krivák

The submitted thesis deals with the structure-based prediction of protein-ligand binding sites with the focus on small ligands. Prediction of such binding sites is central to many applications, including computational drug discovery. The thesis presents a substantial contribution to the field, comprising i) the development of a machine learning method for the detection of binding sites, ii) developing a software tool implementing the ML approach, iii) participation in the development of a web-based solution for binding site prediction and iv) participation of dissemination of the results via the PDBe-KB international community effort.

The problem of protein-ligand binding site prediction has been one of our research group's core research topics, and the thesis's author played a pivotal role in this pursuit. He developed and maintained the core approach for binding site prediction and was involved in almost all research directions stemming from it, such as extending the approach towards different ligand types such as peptides, an already published research, or ions, an ongoing project.

Over the years, Radoslav has shown he is very well capable of independent research, consistently generating innovative ideas not only within his direct research area but

regularly proposing novel research ideas beyond the scope of his domain, proving that he can see the problems in a broader context.

The number of citations of his work and the current widespread adoption of the software attest not only to the candidate's research qualities but also to his expertise in software development.

The candidate has shown that he can carry out his own individual research, come up with and validate new ideas, and work as part of a larger team. I believe that the candidate proved to be able to perform research and achieve scientific results. Therefore, I do recommend the thesis for defense.

doc. RNDr. David Hoksza, Ph.D.