

Virtual screening is a well-established part of computer-aided drug design, which heavily employs similarity search and similarity modeling methods. Most of the popular methods are target agnostic, leaving space for design of new methods that would take into account the specifics of the particular molecular target. Additionally, newly developed methods suffer from two related issues: benchmarking and availability. Benchmarking in the domain often suffers from the use of inappropriate reference methods, lack of reproducibility, and the use of nonstandard benchmark datasets. Although there have been several benchmarking studies in the domain that aim at addressing these issues, mainly by offering a standardized comparison, they often suffer from similar drawbacks. For these reasons, new methods fail to gain trust and therefore fail to become a part of the standard toolbox, which thus consists mostly of older methods. In this work, we address the above-described issues. First, we introduce new adaptive methods for virtual screening. Then, to make our and other newly developed methods readily available, we have designed and implemented a virtual screening tool. To address the benchmarking issue, we have compiled a publicly available collection of benchmarking datasets and proposed a platform offering a reproducible benchmarking environment for virtual screening methods.