Subject: Re: Dealing with multiple "0% inhibition" results in HTS tests
Posted by sansun on Tue, 12 Jul 2022 05:14:15 GMT
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Hi

There are many ways by which you can use the structural information of inactive compounds in medicinal chemistry. You can use these molecules to validate your computational models, e.g. QSAR, pharmacophore, docking protocol, machine learning models etc.

e.g. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3438292/

Your model should be able to pick up active molecules while discard inactive ones.

You can also compare physicochemical properties of inactive and active molecules and find out the chemical space in which the probability of finding active molecules may increase for a particular target.

e.g. https://pubs.acs.org/doi/full/10.1021/acsomega.1c00104

I hope it helps!

SS