INTRODUCTION

The goal in virtual screening, the high-throughput computational evaluation of small molecules as potential protein activators or inhibitors, is to select a small set likely to show activity in experimental tests.

The challenge is to identify features that distinguish a small number of active compounds (typically 10 or fewer) from 100,000s to millions of molecules being screened.

We developed Screenlamp, a computational tool to increase the computational efficiency and success rate in virtual screening and to facilitate hypothesis-driven molecular selection and the analysis of structure-activity relationships using machine learning.

REFERENCES


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