



Drug repurposing is the application of existing drugs for use in a different disease. Such an exercise holds many advantages over traditional drug discovery processes. It reduces the costs and development time and, since these drugs already have successfully passed clinical trials, detailed information on their pharmacology, formulation, dose, and potential toxicity is available. Despite all the benefits, a comprehensive library of compounds that have reached phase 1 clinical trials is not commercially available.

The Broad Institute of MIT and Harvard in Cambridge, Massachusetts, have made a large-scale, systematic effort in building the Drug Repurposing Hub, searching open and proprietary databases for clinically tested drugs. Approximately 10,000 small-molecule drugs with disclosed structures were found to have reached clinical development, but most of these drugs are not widely available for commercial screening. In the end, 5,691 unique compounds were purchased from 75 chemical vendors to assemble the library.

Library details

Specs was able to source most of these compounds, confirm their identity and purity through H-NMR and UPLC and make them available for screening in appropriate pre-plated formats. Initially serving a consortium of 5 drug discovery organisations, a total of 5,632 compounds were plated in 96- and 384-well SBS standard plates for less than €35,- per compound.

This includes compound and data aggregation, supplier shipment costs, QC-analysis and data interpretation (including spectra), reformatting, plating, costs of consumables and dry ice shipment to the end users.

Availability

The Fraunhofer Institute for Molecular Biology and Applied Ecology successfully identified a large number of inhibitors in this library against SARS-CoV-2 in human in-vitro cellular toxicity studies of which 19 showed an $IC_{50} < 1\text{mM}$. We still have a few copies of this pre-plated library as a 10mM DMSO solution in 384-well plates that can be delivered on short notice.

It is also possible to cherry-pick specific compounds from the database and have them shipped in any given format. If you are interested in this repurposing library or wish to receive any additional information, please contact us at info@specs.net