Introduction to the six molecular features supported by Transcell

Six measurement types of data used in Transcell were downloaded from the figshare or DepMap (figshare (data description here): mutation, gene expression, copy number variation, gene effect, drug sensitivity. DepMap: CCLE_RPPA_20181003, CCLE_RPPA_20181003, CCLE_metabolomics_20190502). All the datasets can be downloaded from the compiled RData file. In the RData file:

#octad_cell_line_meta: cell line meta information (including disease type, etc.) #octad_cell_line_features: feature description (including gene name, etc.) #octad_cell_line_matrix: all values

Metabolite:

The method is detailed in the <u>publication</u> (Li et al. *Nature Medicine*, 2019). Note that the abundance of different metabolites cannot be compared given the nature of the LC-MS methods. Only for the same metabolite, the levels could be compared between different cell lines.

Protein:

Data are generated based on the Reverse Phase Protein Array (RPPA) technology, including isoforms and different protein states. Antibodies are listed here in the <u>portal</u>.

Copy number variation (CNV):

Gene level copy number data, log2 transformed with a pseudo count of 1. This is generated by mapping genes onto the segment level calls.

Gene effect score:

The DepMap released data containing CRISPR knockout screen results from the project Achilles. A lower score means a high gene dependency (DepMap used -1 as a threshold to define the dependency).

Drug Sensitivity:

The primary PRISM Repurposing dataset contains the results of pooled-cell line chemical-perturbation viability screens for >4,500 compounds screened against >550 cell lines. The data used in Transcell are logfold change values which are relative to DMSO and corrected for experimental confounders using ComBat. The more negative a value is, the more effective the compound is in the corresponding cell line.

Mutation:

We define 1: mutated, 0: wild, NA: unknown (NA for those cell lines which do not have mutation profiles). The following mutation types listed in Variant_Classification were ignored: 3'UTR", "Intron", "5'UTR", "plice_Site_SNP", "Silent", "De_novo_Start_OutOfFrame", "De_novo_Start_InFrame", "Unknown", "Substitution - coding silent", "No detectable mRNA/protein".