

Screen and cell line specific variables

Variable	Explanation
BARCODE	Barcode of screening plate
CELL_LINE_NAME	Cell line name
COSMIC_ID	COSMIC Identifier
SIDM	Cell Model Passports identifier
TISSUE	Tissue
CANCER_TYPE	Cancer type
MSI_status	Microsatellite instability (MSI = instable, MSS = stable)

Anchor-specific variables

Variable	Explanation
ANCHOR_ID	Sanger Drug ID for anchor drug
ANCHOR_NAME	Name of anchor drug
ANCHOR_TARGET	Targets of anchor drug
ANCHOR_PATHWAY	Pathways of anchor drug targets
ANCHOR_GENE_TARGET	Targets of anchor drug, expressed in gene names
ANCHOR_DRUG_TYPE	Information whether the anchor drug is a chemotherapeutic or targeted compound
ANCHOR_CONC	Concentration of anchor drug in $\mu\text{M}$
ANCHOR_VIABILITY	Viability of the anchor drug
ANCHOR_VIABILITY_SD	Standard deviation of anchor viability

Library-specific variables

Variable	Explanation
LIBRARY_ID	Drug ID for library drug
LIBRARY_NAME	Name of library drug
LIBRARY_TARGET	Targets of library drug
LIBRARY_PATHWAY	Pathway of library drug targets
LIBRARY_GENE_TARGET	Targets of library drug, expressed in gene names
LIBRARY_DRUG_TYPE	Information whether the library drug is a chemotherapeutic or targeted compound
LIBRARY_CONC	Highest used library concentration
LIBRARY_SCAL	Scale used for dose points for library drug
LIBRARY_RMSE	RMSE (root mean square error) of library response curve
LIBRARY_XMID	Concentration of library drug that reduces viability by 50%, log2 scale with -1 to 9 representing the screening range
LIBRARY_XMID_uM	Concentration of library drug that reduces viability by 50%, in $\mu\text{M}$
LIBRARY_EMAX	Emax (viability at the highest used concentration) of the library
LIBRARY_AUC	Area under curve of library, calculated using trapezoid approximation
LIBRARY_fAUC	Area under curve of library, calculated using integral of library response curve

Drug combination-specific variables

Variable	Explanation
SYNERGY_RMSE	RMSE (root mean square error) of combination response curve
SYNERGY_XMID	Concentration of library drug to the combination that reduces viability by 50%, log2 normalised scale with -1 to 9 representing the screening range
SYNERGY_DELTA_XMID	$\Delta IC50 = LIBRARY\_XMID - SYNERGY\_XMID$ , log2 normalised scale
SYNERGY_XMID_uM	Concentration of library drug to the combination that reduces viability by 50%, in uM
SYNERGY_DELTA_XMID_uM	$\Delta IC50 = LIBRARY\_XMID\_uM - SYNERGY\_XMID\_uM$ , in uM
SYNERGY_EXP_EMAX	Expected Emax (viability at the highest used concentration) of the combination based on Bliss formula, 0-1 viability scale
SYNERGY_OBS_EMAX	Observed Emax (viability at the highest used concentration) of the combination, 0-1 viability scale
SYNERGY_DELTA_EMAX	$\Delta Emax = SYNERGY\_EXP\_EMAX - SYNERGY\_OBS\_EMAX$ , -1 to 1 viability scale
SYNERGY_OBS_AUC	Area under curve of expected (Bliss) combination, calculated using trapezoid approximation
SYNERGY_EXP_AUC	Area under curve of observed combination, calculated using trapezoid approximation
SYNERGY_DELTA_AUC	$\Delta AUC = SYNERGY\_EXP\_AUC - SYNERGY\_OBS\_AUC$
SYNERGY_EXP_fAUC	Area under curve of expected (Bliss) combination, calculated using integral of combination response curve
SYNERGY_OBS_fAUC	Area under curve of observed combination, calculated using integral of combination response curve
SYNERGY_DELTA_fAUC	$\Delta fAUC = SYNERGY\_EXP\_fAUC - SYNERGY\_OBS\_fAUC$
SYNERGY_ZSCORE	$(LIBRARY\_XMID - SYNERGY\_XMID) / replicate\_variance$ . N.B. Replicate variance is a single value per screen

Synergy variables

Variable	Explanation
Pass_dIC50	Does the measurement pass the $\Delta IC50$ synergy threshold, $SYNERGY\_DELTA\_XMID \geq 3$ (corresponds to 8-fold shift)
Pass_dEmax	Does the measurement pass the $\Delta Emax$ synergy threshold, $SYNERGY\_DELTA\_EMAX \geq 0.2$
Synergy	Is the measurement classified as synergistic