How to interpret curve-fitting results

* IC50: if ic50\_label == ‘INSIDE\_TESTED\_RANGE’, use these values.
* IC50: if ic50\_label ==‘OUTSIDE\_TESTED\_RANGE’, preferably cap the IC50 value to the maximum tested concentration (CONC9).
* IC50: if ic50\_label == ‘NO\_VALUE’ use NaN, as in this case the model fits a curve but the bottom of the curve is greater than 0.5, which translates into no possible IC50 value; usually this behavior is due to a very flat (no response) type of curve, well above the viability = 0.5 level.
* Slope sign: if slope\_sign == ‘POSITIVE’, ignore these IC50/EC50/AUC values, as it does not fit the usual drug response behavior (we expect a negative slope in the curve response). For most of these scenarios, you may notice IC50 and EC50 with really low values (unnatural), due to the positive curve-fitting slope.
* Type of fit: if fit == ‘LINEAR’, I would not trust the IC50 values that much, as we would not really fit a logistic curve through this response. You can also see that the IC50 and EC50 are rather unusually high in these cases.

Meaning of column names in the output file (refit\_\*.txt):

* index\_rem = indicates the drug response (percent viability) position that has been removed as a result of outlier removal analysis. During this analysis we simply remove one drug concentration, the value that is the furthest away from the actual curve fit and then retrain the model. The index of that value is indicated by index\_rem.
* residual\_rem = the value of the outlier removed from the above described analysis.
* overall\_residual = the overall residual, computed across all drug concentrations.
* fit\_rem = type of fit (LL4, LL5, LINEAR) after residual removal.
* slope\_sign\_rem = slope of the curve fit, after residual removal.
* ic50\_label\_rem = as above, but after outlier removal.
* overall\_residual\_rem = the overall residual, computed across all drug concentrations, after outlier removal.
* CellsPerWell = cell count, as in seeding concentration.
* ic50\_capped = capped IC50 values.
* ic\_lethal = drug concentration needed to produce a cell population kill at the level of the original seeding density.
* auc = area under the curve, after curve fit.
* auc\_original\_conc = area under the curve, from the original drug response points (area of the polygon created from the x axis and the drug response values).
* ec50 = EC50 estimated values (this is also a parameter in the four/five parameter logistic function).
* top = parameter from the curve fitting algorithm which, in the case of a logistic fit indicates the upper limit of the four/five parameter logistic curve. In the case of a linear fit it becomes NaN.
* bottom = parameter from the curve fitting algorithm which, in the case of a logistic fit indicates the lower limit of the four/five parameter logistic curve. In the case of a linear fit it becomes NaN.
* hs = hill slope of the logistic/linear fit.
* ic50\_rem = estimated IC50 values, after residual removal.
* ic50\_capped\_rem = capped IC50 values, after residual removal.
* ic\_lethal\_rem = drug concentration needed to produce a cell population kill at the level of the original seeding density, after residual removal.
* auc\_rem = area under the curve, after curve fit, after residual removal.
* auc\_original\_conc\_rem = area under the curve, from the original drug response points (area of the polygon created from the x axis and the drug response values), after residual removal.
* top\_rem = parameter from the curve fitting algorithm which, in the case of a logistic fit indicates the upper limit of the four/five parameter logistic curve, after residual removal. In the case of a linear fit it becomes NaN.
* bottom\_rem = parameter from the curve fitting algorithm which, in the case of a logistic fit indicates the lower limit of the four/five parameter logistic curve, after residual removal. In the case of a linear fit it becomes NaN.
* hs\_rem = hill slope of the logistic/linear fit, after residual removal.
* ec50\_rem = estimated EC50 values, after residual removal.