**Supplemental Material and Methods**

*Normalization*

Raw data for the 80 compounds were normalized to the dimethylsulfoxide (DMSO) solvent control wells, by concentration level, as follows. The means and standard deviations of data from DMSO control wells for each endpoint and each concentration level were calculated. Outlier values of the DMSO controls were removed. Outliers in this case are values which differ by more than three times the standard deviation from the mean (for each endpoint/concentration level combination). After outlier removal, the means and standard deviations were recalculated. Normalized values of the data for the 80 compounds were calculated by dividing the raw data by the mean of the DMSO controls for that endpoint and concentration level. Normalized values of the DMSO control data were calculated in the same way. The normalized control data for each endpoint at all concentration levels were pooled, and the standard deviation of the pooled values was calculated.

*Curve fitting*

We modeled the 80 compounds using two functions: The Hill function and the logistic function. The Hill function provided a better fit to the data, as compared to the logistic function, and was therefore used for future analyses.

Outlier-detection algorithm

For each concentration response curve (normalized concentration-response data for one endpoint for one compound), the following procedure was used to detect outliers.

1. The Hill model is used to fit the data, with parameters optimized as described in the main text.

2. Candidate outlier points are found. A point is considered as a candidate if the residual (difference between the fitted model and the data) for that point is at least three times the standard deviation of the pooled DMSO controls for that endpoint. If any such candidate points are found, the procedure goes on to step 3. Otherwise, there are no outlier points to be found.

3. For each candidate point, a reduced data set consisting of all points in the data set except for the candidate point is generated. The standard deviation of the reduced data set is calculated, using the optimized fitted model from step 1, as, where the summation is over points *i* in the reduced data set, *yi* are the data, *fi* are the fitted model values, and *m* is the number of points in the reduced data set.

4. For each candidate point, the log-likelihood of the optimized parameters from step 1 for the reduced data set is calculated using the likelihood function for a normal distribution:

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5. For each candidate point, the model is refitted to the reduced data set, using the same optimization procedure and limits on parameter values as described previously. The standard deviation and likelihood are calculated as above, but using the model values from this refit. The likelihood from this refit will be referred to as *L2*.

6. The ratio *R*=*L2*/*L1* is calculated for each candidate point. This ratio describes the improvement in the fit to the other data points when the candidate outlier point is removed from the data. If there are candidate points for which *R* > 10, those points are kept as candidate points and the procedure goes on to step 7. Otherwise, there are no outlier points to be found.

7. In these data sets, each compound is measured in duplicate at each concentration. It is possible that very different values of the duplicates may be due to true variation in the response, rather than one of the values being an outlier. In particular, it is possible for a compound to show nearly no response below a given concentration (responses are near the control value of 1), and strong responses (typically as part of a decreasing curve, with values <1) above that concentration, with one of the two responses at the intermediate concentration being weak (near the control value of 1) and the other being closer to the response at higher concentrations. In this case, removing either one of the other duplicate responses will make it possible for the model to give a good fit to the other duplicate. In this situation, we assume that neither of the two responses should be considered an outlier.

The algorithm deals with this possibility as follows. For each outlier candidate from step 6, if the duplicate point at that same concentration has not been already marked as an outlier, then a second reduced data set is generated by removing the duplicate point from the data. Then, the model is fitted to the second reduced data set as described above. If this model fit has a residual for the original outlier point of less than three times the standard deviation of the pooled DMSO controls, then removing the duplicate has given a good model fit to the candidate point, which is therefore no longer considered an outlier candidate. If any outlier candidates remain after this calculation has been carried out, then the procedure goes on to step 8. Otherwise, there are no outlier points to be found.

8. From the set of all remaining candidate points, the one with the highest ratio *R* from step 6 is chosen as an outlier. The whole procedure is done again, starting at step 1, with the outlier point removed from the data used for the fit. This is repeated until no further outlier points are found.