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Supplementary Material

Lessons learned from evaluating defined chemical mixtures in a high throughput estrogen receptor assay system

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Files in S4\_FitAndModelPlots.zip:

The files named [assay name]\_HillFunctionFits.pdf contain data and Hill function fits from the two assays (ER-bla and ER\_luc). Black circles are data. Circles with black outlines only are data omitted from the curve fit. Solid black lines are fit to the data. Dashed black lines are the confidence limits of the fit. The x-axis in plots of mixture data is the total concentration of all mixture components.

For the ER-luc assay in ER-luc\_HillFunctionFits.pdf the abbreviation of mix indicates when the mixture driven by zearalenone was used as a proxy for estimating the zearalenone concentration-response curve was used (see the Methods section).

The files named [assay name]\_[model name].pdf contain data, fits, and predictions of the named model for the named assay. Black circles are data. Circles with black outlines only are data omitted from the curve fit. Solid black lines are fit to the data. Dashed black lines are the confidence limits of the fit. Solid red lines are mixture model predictions. Dashed red lines are their confidence limits. Other colored lines are responses of mixture components at the concentrations at which they occur in the mixture. Only components with maximum predicted response equal to at least 5% of positive control are plotted. The x-axis is the total concentration of all mixture components.

Data, Hill function fits, and model predictions are values after subtracting the fitted value for response at control concentration (the parameter f0 in the Hill function).