New Features of KinTek Explorer Version 6.0

Windows 10 compatibility. Version 6.0 has been adapted to be compatible with Windows 10. Our tests indicate that the odd problems seen with Windows 7 on a minority of computers have been solved.

Mac OSX 10.12 compatibility. Version 6.0 solves the problems seen on some Mac computers.

Direct output of publication quality EPS and PNG files. In exporting the simulation fitting, we now generate a publication quality EPS vector graphics file. You can now go straight from fitting to publication without the tedious and time consuming process of inputting data and formatting a figure for publication using an external graphics program. If necessary, the EPS file can be directly edited or combined into a composite figure using Adobe Illustrator. In addition to the simulation based fitting results, you can output the results from fitting to analytic functions, and the results of SVD analysis in fitting time-resolves spectra, including 3D plots of the spectra. This feature is available only in the Professional version of the software. Student assignments can use screen capture. *Note if you are using Windows, you will need to install Python to take advantage of this new feature. See installation notes*.

Fitting to define starting concentrations. We have enabled a new function to allow the starting concentrations of reactants to vary in the process of fitting. You can limit the allowed range of variation to a fixed percentage. This is useful to account for slight errors in pipetting to make up solutions or to solve for unknown enzyme concentrations.

Labeled/Unlabeled reactants. We have added functions to allow easy entry of parallel reactions for labeled and unlabeled reactants. See ribozyme.mec for an example involving the use of fluorescently labeled and unlabeled oligonucleotide binding to a ribozyme. Use the **^ symbol** *after* the species name in the *Model Editor* to designate labeled and unlabeled variants of the same species. The program then creates two parallel sets of reactions with identical rate constants.

Lettered rather than numbered linked rate constants. We expanded the number of linked rate constants from 9 to 26 by switching from number 1-9 to letters a-z.

Rate or Amplitude versus Concentration Plots. In fitting data to analytic functions for a concentration series, it is useful to plot rate and amplitude versus concentration to infer the underlying mechanism. However, at the extremes of high or low substrate concentration, fitting often returns values with large errors and this throws off the plots. Now with Version 6.0 you can eliminate points from the figure to reveal the concentration dependence from the reliable data. Just *Shift-click* on a data point on the plot and it will be removed and the plot rescaled. For a good example of this, see PNPase-Pf-DADMe-ImmH.mec and use *aFit* with a burst equation. At low and high inhibitor concentration, it is not possible to obtain reliable fits to the burst equation due to the errors inherent in fitting data to multiple exponentials. In conventional fitting these data must be excluded–that is why we fit globally using simulation where all of the data can be included!

SPR Data Fitting. We have made an initial effort to fit data obtained by SPR (surface plasmon resonance) by allowing "mix-steps" to specify a new fixed concentration that is not consumed by the reaction since it replenished by the continuous flow. That is, with each new phase of SPR, the concentration of the reactant (analyte) is specified by the concentration in the flowing solution. Use the syntax: **[%n]** where n is the new concentration (brackets dictate that the concentration remains constant). Without the brackets, **@n** specifies a new concentration, forgetting the concentrations carried over from previous steps. *There are still serious limitations in fitting SPR data rigorously because of complications due to mass transfer and surface density of receptors, leading to correction factors that are often larger than the signal!*

SVD analysis of equilibrium titrations. Spectra collected as a function of a titration, including pH dependence, can now be fit using SVD analysis to resolve component spectra. This is illustrated by the pH dependence of absorption and fluorescence spectra. As part of this, we enabled the use of *log scales* in titrations.

Repetitive reactions. It is now easier to enter multiple reactions in sequence with linked rate constants. For example, you can easily program 100 sequential reactions for DNA polymerization or actin nucleation and polymerization.