

KinTek Global Kinetic Explorer

New! Dynamic Kinetic Simulation and Global Data Fitting Software
For PC, MAC and Linux

Features...

Simple, intuitive user interface: Enter new models in simple $E + A = EA = EI = EP = E + P$ format, with instant feedback to highlight errors while you type

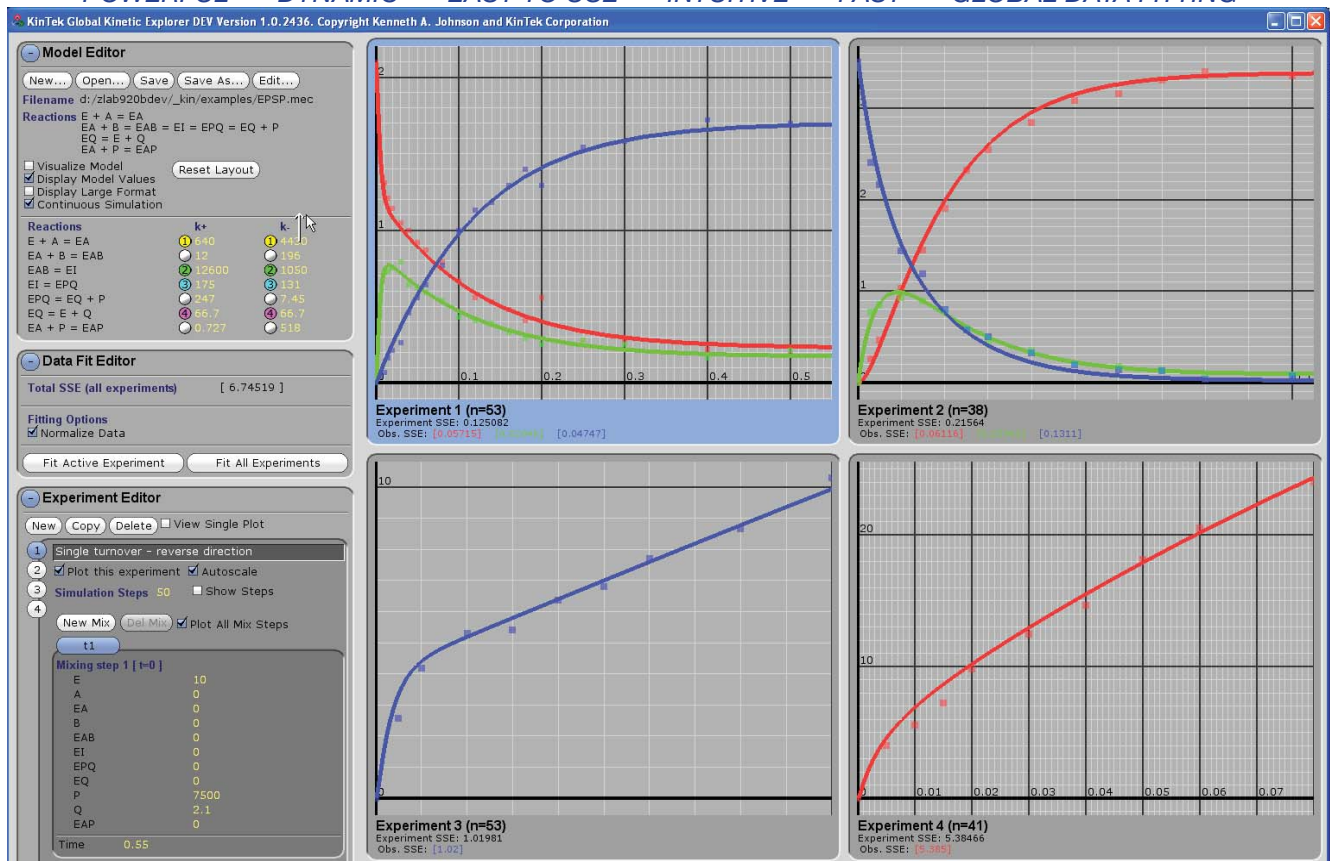
Dynamic simulation: Scroll rate constants, starting concentrations and output factors while viewing changes in the shape of the graph

Robust data fitting routines: Perform nonlinear regression based upon the simulation model, not mathematical approximations to reality

Global Fitting of multiple experiments: Simultaneously fit multiple experiments performed under different starting conditions

Exploration using linked or fixed rate constants: Fix individual constants or link two or more rate constants to vary in unison while dynamically scrolling and fitting data

POWERFUL ♦ DYNAMIC ♦ EASY TO USE ♦ INTUITIVE ♦ FAST ♦ GLOBAL DATA FITTING



Screenshot showing global fitting of four experiments performed on EPSP synthase and fit simultaneously.

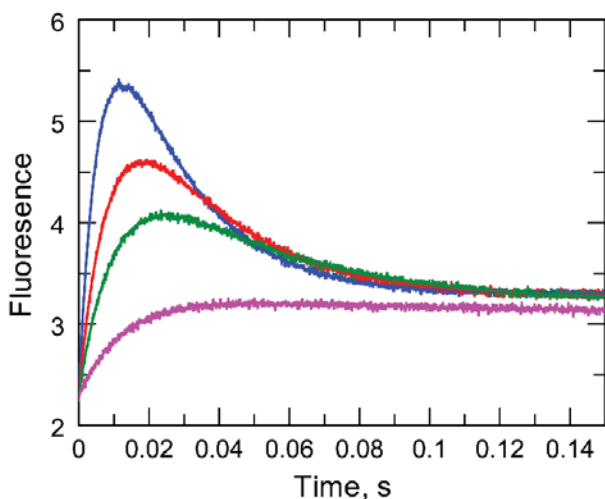
Benefits...

The *Fast Dynamic Simulation and Intuitive user interface* make it easy to compare multiple models and to explore relationships between the kinetic parameters and the observable outputs. Seeing the curves change in shape as you scroll a rate constant or starting concentration provides immediate feedback to learn kinetics, evaluate models, and explore whether any constant is determined by the data. Moreover, *Global Data Fitting* directly to the model eliminates the tedious and error-prone analysis using conventional methods that depend upon fitting to simplified mathematical models. Simultaneously fitting multiple experiments constrains the fit and ensures that the model quantitatively accounts for all of the data, and the ability to link or fix rate constants further ensures that the fitting of data to the model is sufficiently constrained to be meaningful.

KinTek Global Kinetic Explorer offers unprecedented power to design and rigorously interpret experiments to fully unleash your creative potential!



Advantages of Fitting Data Directly to the Model by Simulation



**Conventional
Data Fitting**

**KinTek Explorer
Data Fitting**

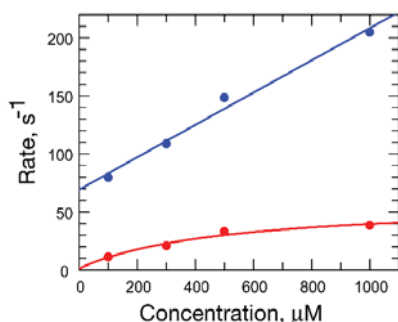
1. Derive equation for time dependence

$$Y = A_1 \cdot e^{-\lambda_1 t} + A_2 \cdot e^{-\lambda_2 t} + C$$

2. Fit data to extract rates

[S]	λ_1	λ_2
100	10	79
30	18	112
500	30	141
1000	41	204

3. Replot rates versus concentration

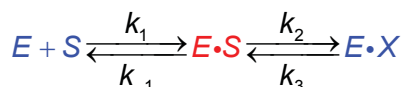


4. Derive equations for rate vs concentration

$$\lambda_1 \approx k_1[S] + k_{-1} + k_2 + k_{-2}$$

$$\lambda_2 \approx \frac{k_1[S](k_2 + k_{-2}) + k_{-1}k_{-2}}{k_1[S] + k_{-1} + k_2 + k_{-2}}$$

5. Fit equation to extract rate constants



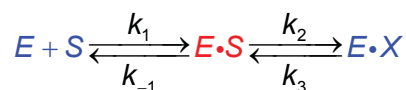
Net: You fit data to 24 unknown parameters and get estimates for only 3 rate constants. An estimate for the four constant, k_{-2} , depends upon additional analysis of reaction amplitudes.

1. Enter model and define output



$$Fluor = f_0 + f_1 \cdot [ES]$$

2. Globally fit rates to model



Net: You fit data to obtain reliable estimates for all 4 rate constants and 2 fluorescence output factors in one step.

Conventional data fitting requires simplifying assumptions to allow mathematical solutions of equations describing a chosen model, followed by fitting to analytical functions, replotting of observed rates and extraction of rate constants according to the assumed model.

With the release of *KinTek Global Kinetic Explorer*, conventional methods of data fitting are obsolete! Fitting data directly to the model based upon simulation is easier and more accurate.

In the *New Enzymology*, even steady state data should be fit globally to the model, bypassing the steady state assumption and all of the equations.

Benefits of Global Data Fitting

- Faster and more accurate fitting
- No simplifying assumptions
- No errors in deriving equations
- No need for pseudo-first order conditions
- Alternative models can be evaluated
- Dynamic simulation gives feedback