Small Molecular, Macromolecular and Cellular Chloramines React with Thiocyanate to Give the Human Defense Factor Hypothiocyanite

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SUPPORTING INFORMATION

Mathematica code used to fit the data of Figure 3.

```
Do[

    Clear[h, nsteps, TauCl, SCN, OSCN, Prod, k1, k2, data];

    SCN = 0.01;
    totaltime = 5;
    h = 0.01;
    nsteps = Round[totaltime/h];
    k1 = 100;
    k2 = 5000;
    TauCl[0] = TauClZero;
    OSCN[0] = 0;
    Prod[0] = 0;

    Do[
        {
         TauCl[n] = TauCl[n - 1] - h*k1*TauCl[n - 1]*SCN,
         OSCN[n] = OSCN[n - 1] +  h*k1*TauCl[n - 1]*SCN -  h*k2*TauCl[n - 1]*OSCN[n - 1],
         Prod[n] = Prod[n - 1] + h*k2*TauCl[n - 1]*OSCN[n - 1]
         },
    {n, 1, nsteps, 1}] // N;

    data = Table[{TauCl[n], OSCN[n], Prod[n]}, {n, 0, nsteps}];

    (* Include the following to plot concentration vs. time

    TableForm[data];
    datatr=Transpose[data];
    TauClt=ListPlot[datatr[[1]], DisplayFunction -> \
   Identity,PlotStyle->Red]
    OSCNt=ListPlot[datatr[[2]], DisplayFunction -> \
   Identity,PlotStyle->Blue]
    Prodt=ListPlot[datatr[[3]], DisplayFunction -> \
   Identity,PlotStyle->Green]

    Show[{ TauClt, OSCNt, Prodt},  DisplayFunction -> $DisplayFunction]
    *)

    Print["[TauCl]0 = ", TauClZero];
    Print["Final Concentration OSCN = ", OSCN[nsteps - 1]];
    Print["Percent Yield = ", 100*OSCN*[nsteps - 1]/TauClZero];
    Print["++++++++++++++++++++++++++++++++++++++++++++++++++"],

{TauClZero, 0.00025, 0.002, 0.00005}]
```

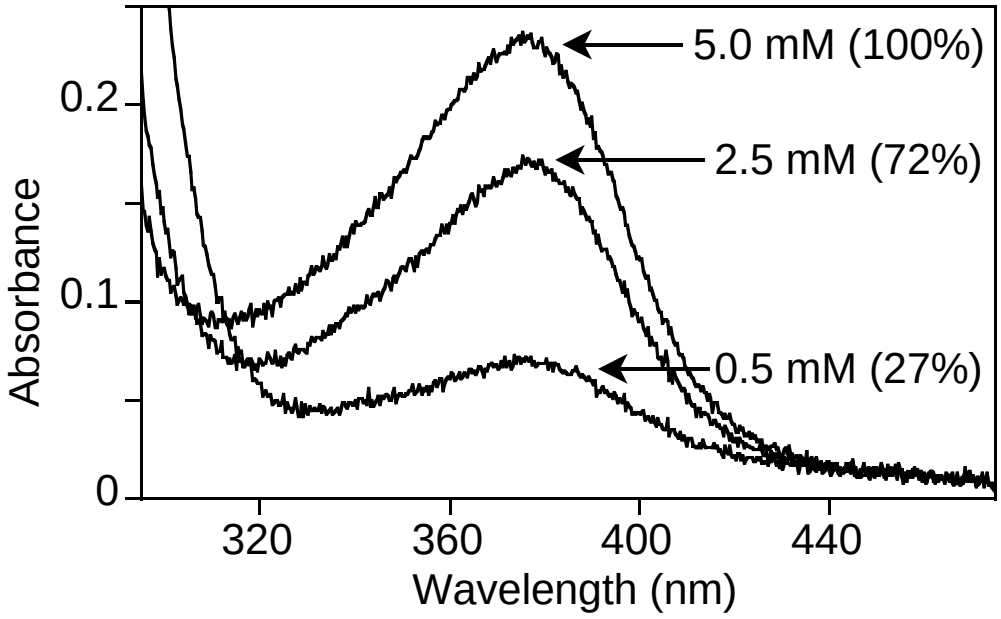

Figure S1. UV-vis spectra obtained for the reactions of TauCl (80 μM) with SCN^- (0.5-5.0 mM) in phosphate buffer (100 mM, pH 7.4). The spectra were recorded with a 1 meter fiber optic cell. The chemical yield of $OSCN^-$ is indicated versus $[SCN^-]_0$.

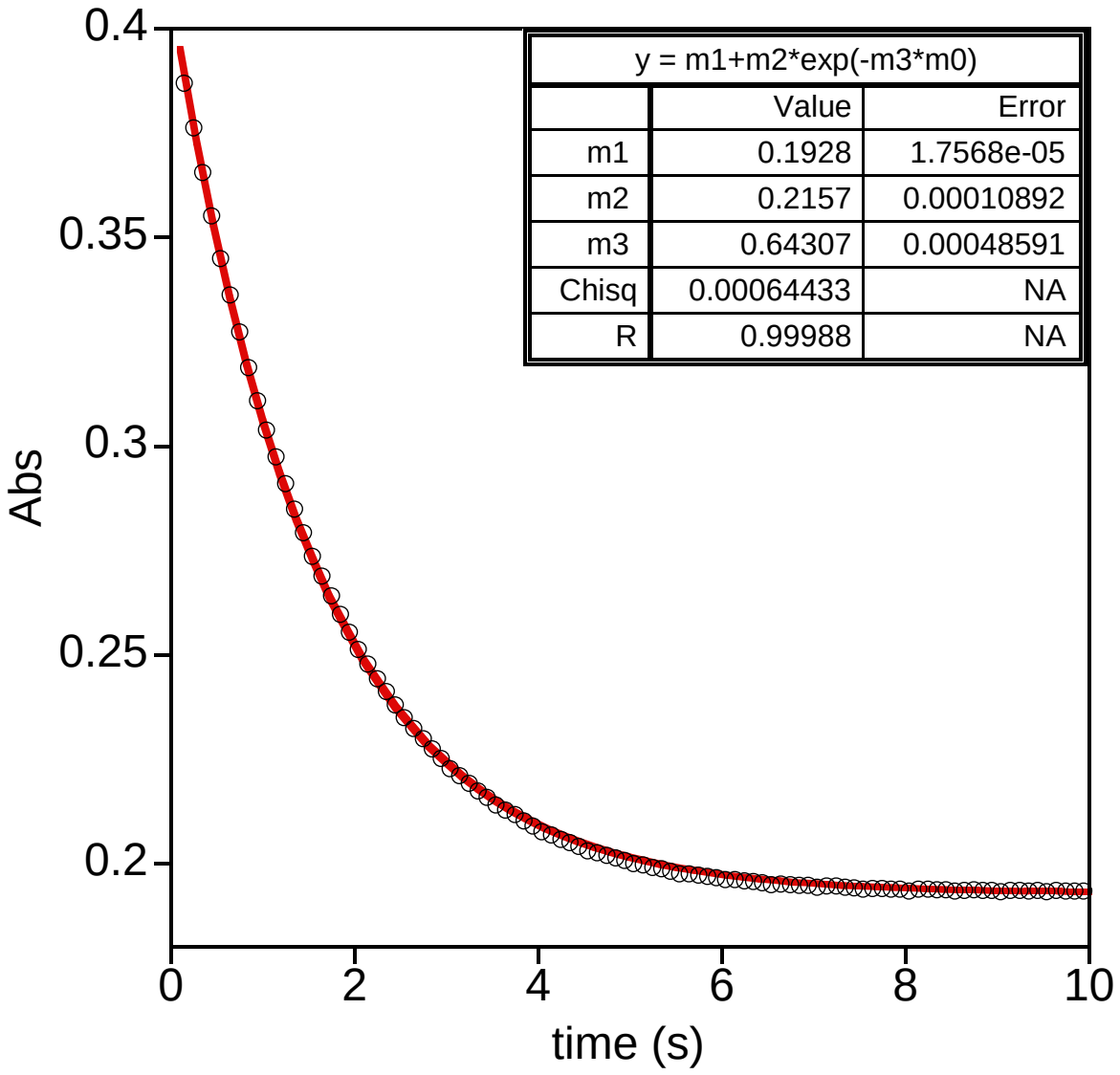

Figure S2. Observed absorbance decrease at 250 nm for the reaction of TauCl (0.5 mM) with SCN^- (5 mM) at pH 7.4 and I = 1.0 M. A first-order fit (red) and 10% of the data (black circles) are illustrated.

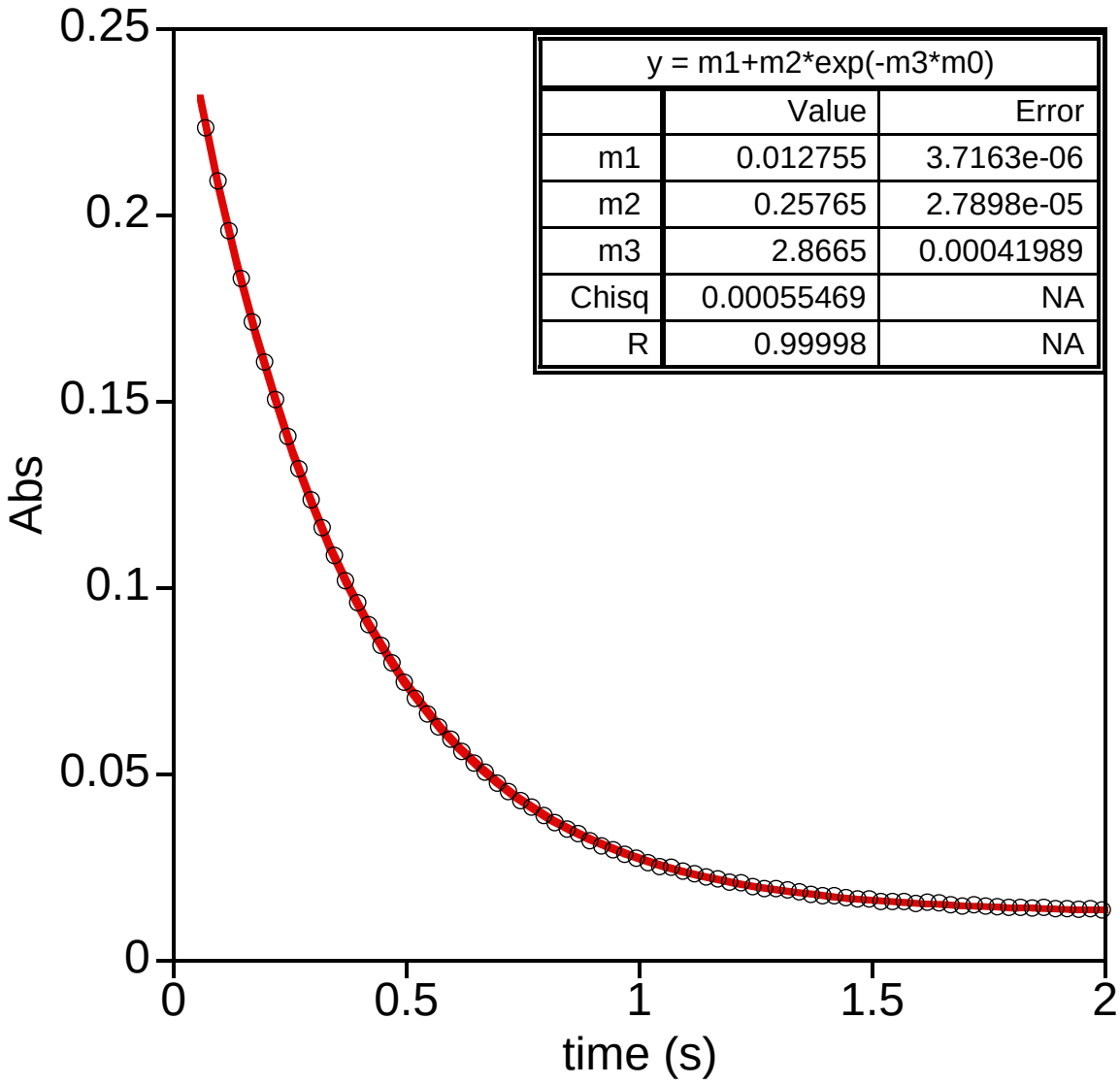

Figure S3. Observed absorbance decrease at 412 nm for the reaction of TauCl (208 μM) with TNB (16 μM) at pH 7.4 and I = 1.0 M. A first-order fit (red) and 2% of the data (black circles) are illustrated.

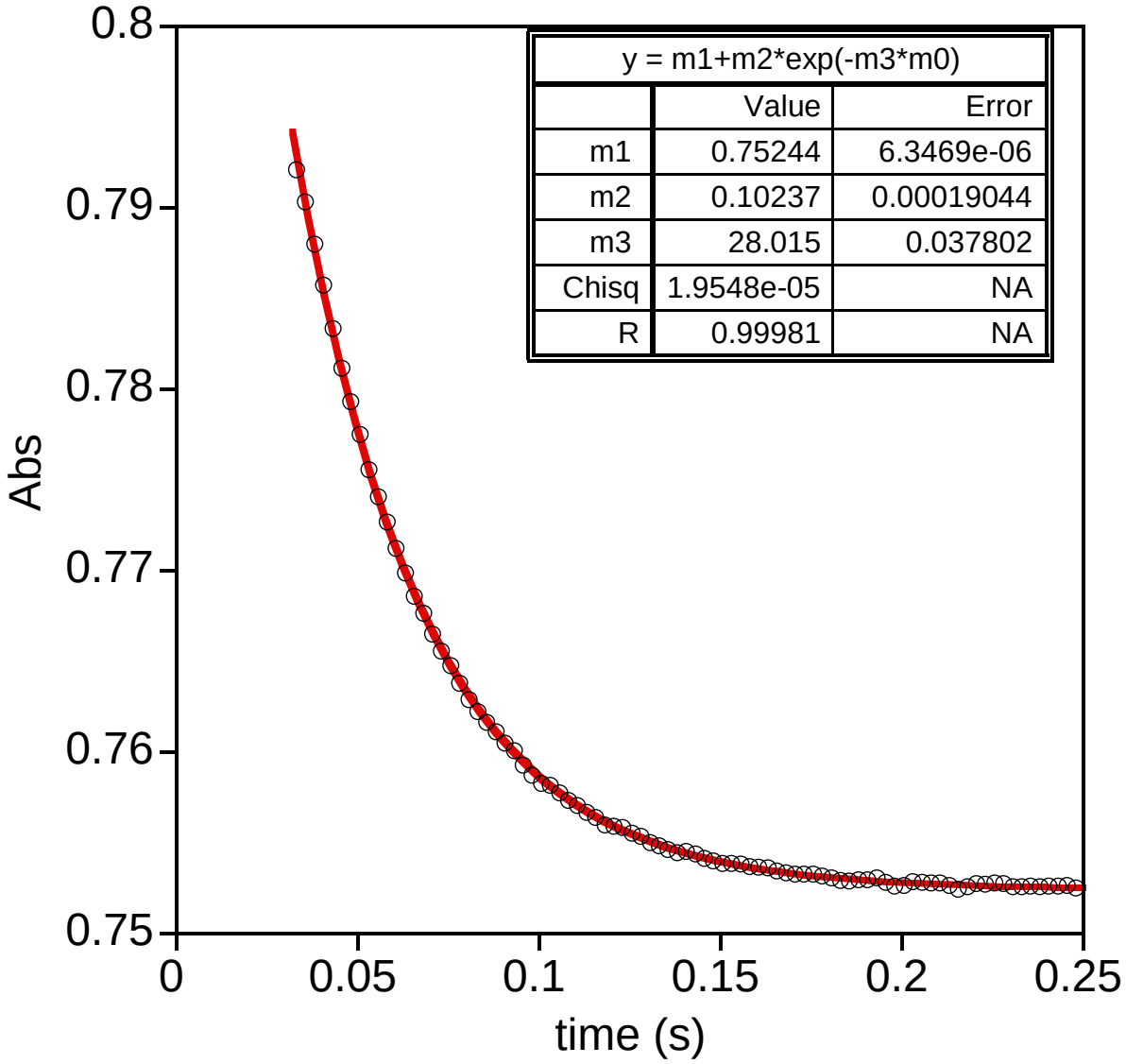

Figure S4. Observed absorbance decrease at 412 nm for the reaction of $OSCN^-$ (4 μM, produced by the LPO-catalyzed oxidation of SCN^- by H_2O_2) with TNB (56 μM) at pH 7.4 and I = 1.0 M. A first-order fit (red) and 20% of the data (black circles) are illustrated.

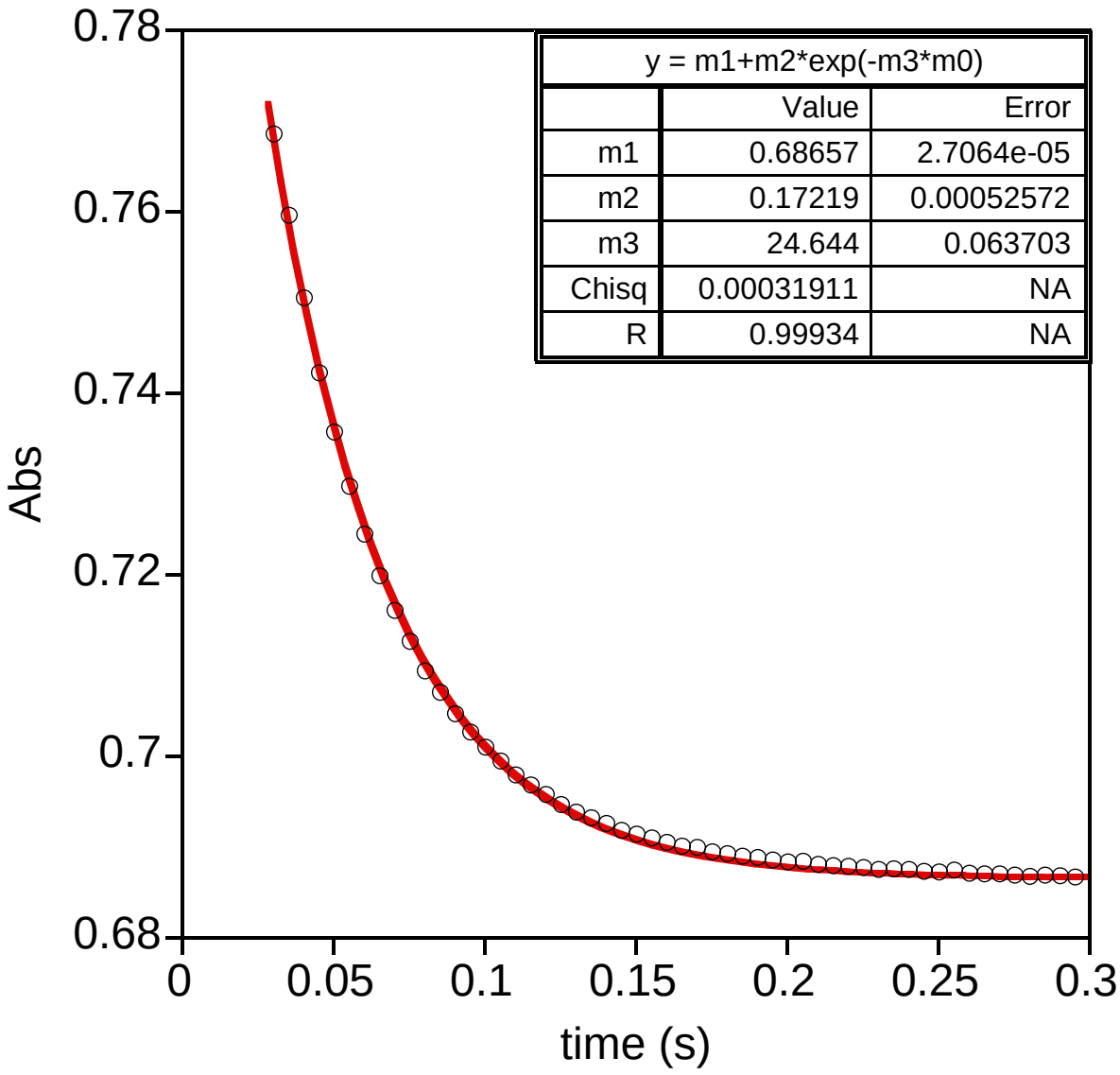

Figure S5. Observed absorbance decrease at 412 nm for the reaction of $OSCN^-$ (5.5 μM, produced by the uncatalyzed oxidation of SCN^- by TauCl) with TNB (56 μM) at pH 7.4 and I = 1.0 M. A first-order fit (red) and 10% of the data (black circles) are illustrated.

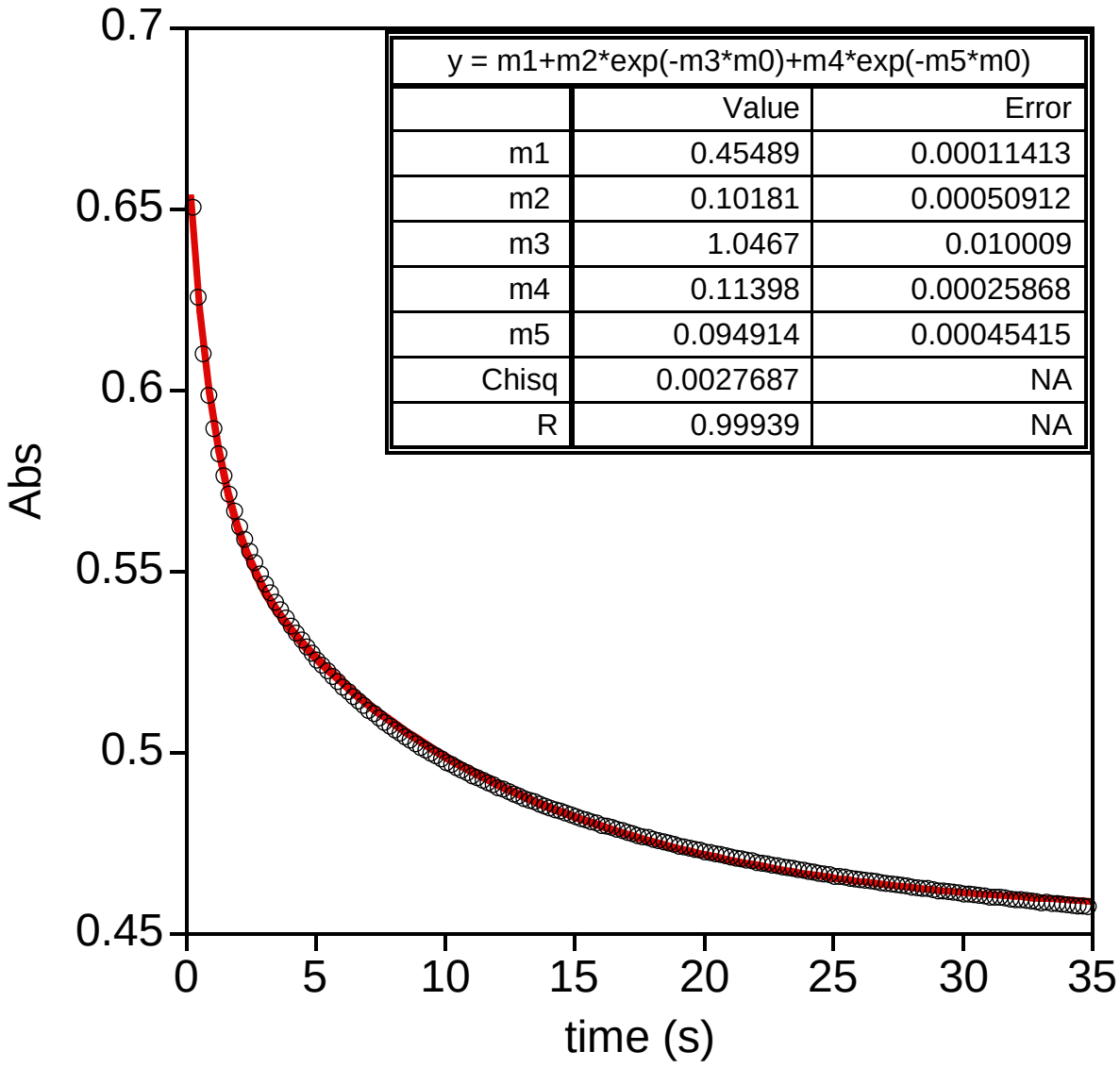

Figure S6. Observed biexponential (decrease-decrease) absorbance decrease at 412 nm for the reaction of Ub*Cl (6 μM, based upon the amount of HOCl used) with TNB (68 μM) at pH 7.4 and I = 1.0 M. A biexponential fit (red) and 10% of the data (black circles) are illustrated.

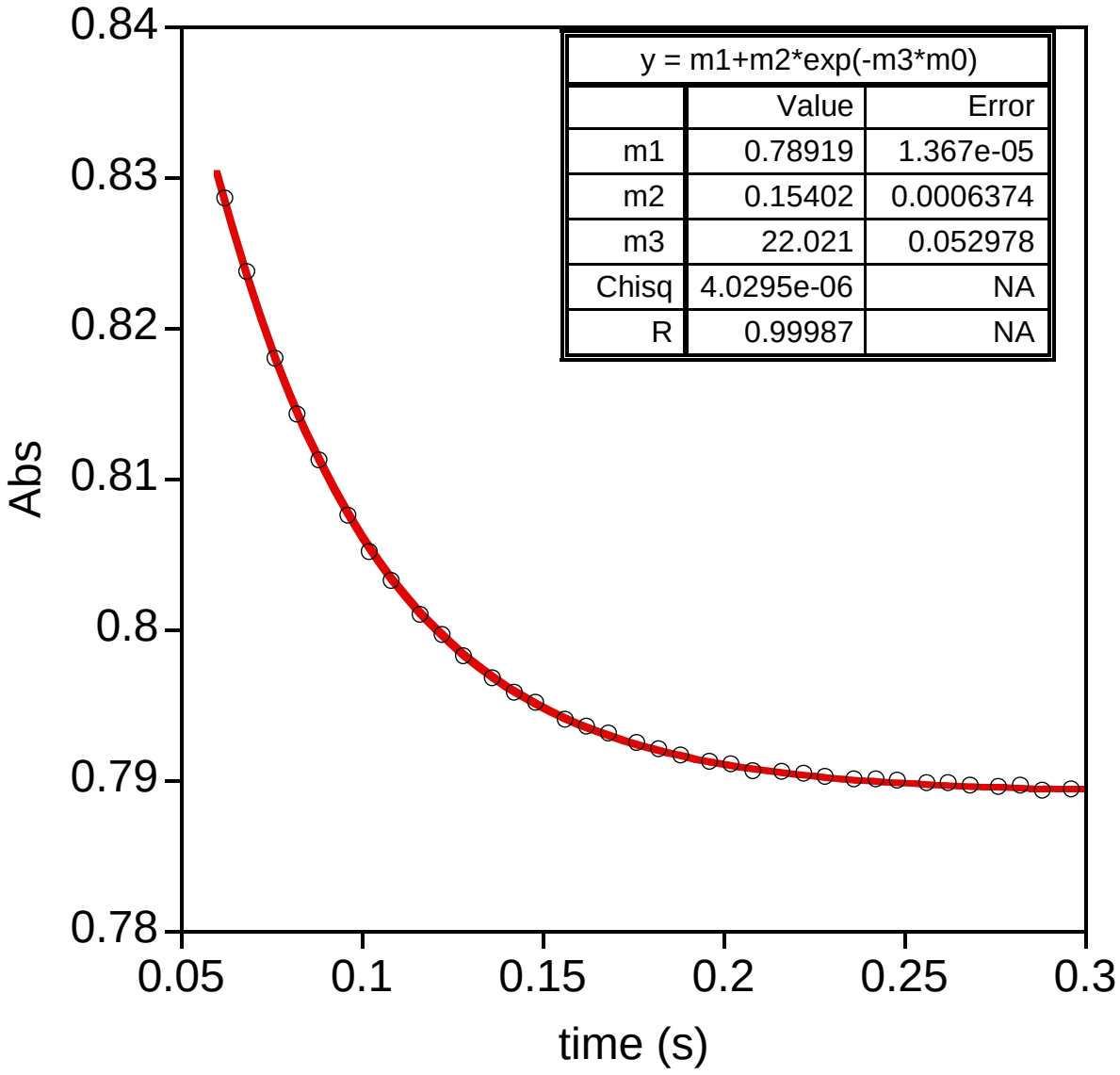

Figure S7. Observed absorbance decrease at 412 nm for the reaction of Ub*Cl (6.75 μM) with SCN^- (0.5 mM) for 20 minutes, followed by reaction with TNB (58.66 μM) at pH 7.4 and I = 1.0 M. A first-order fit (red) and 10% of the data (black circles) are illustrated.

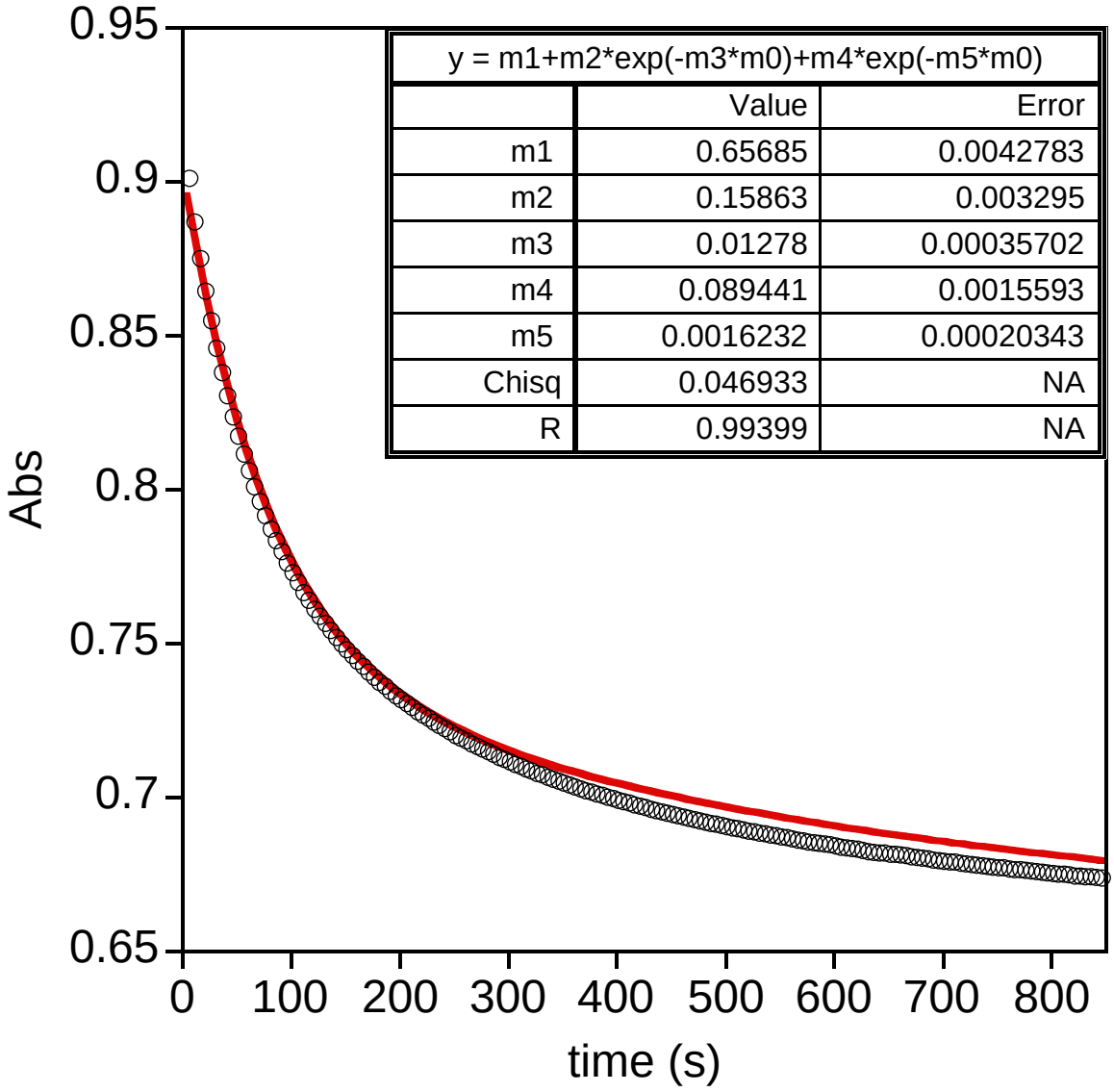

Figure S8. Absorbance decrease at 412 nm for the reaction of chlorinated *E. coli* (6 μM, based upon the HOCl used) with TNB (60.8 μM) at pH 7.4 and I = 1.0 M. A biexponential fit (red) and 10% of the data (black circles) are illustrated. The kinetic trace is apparently multi-phasic.

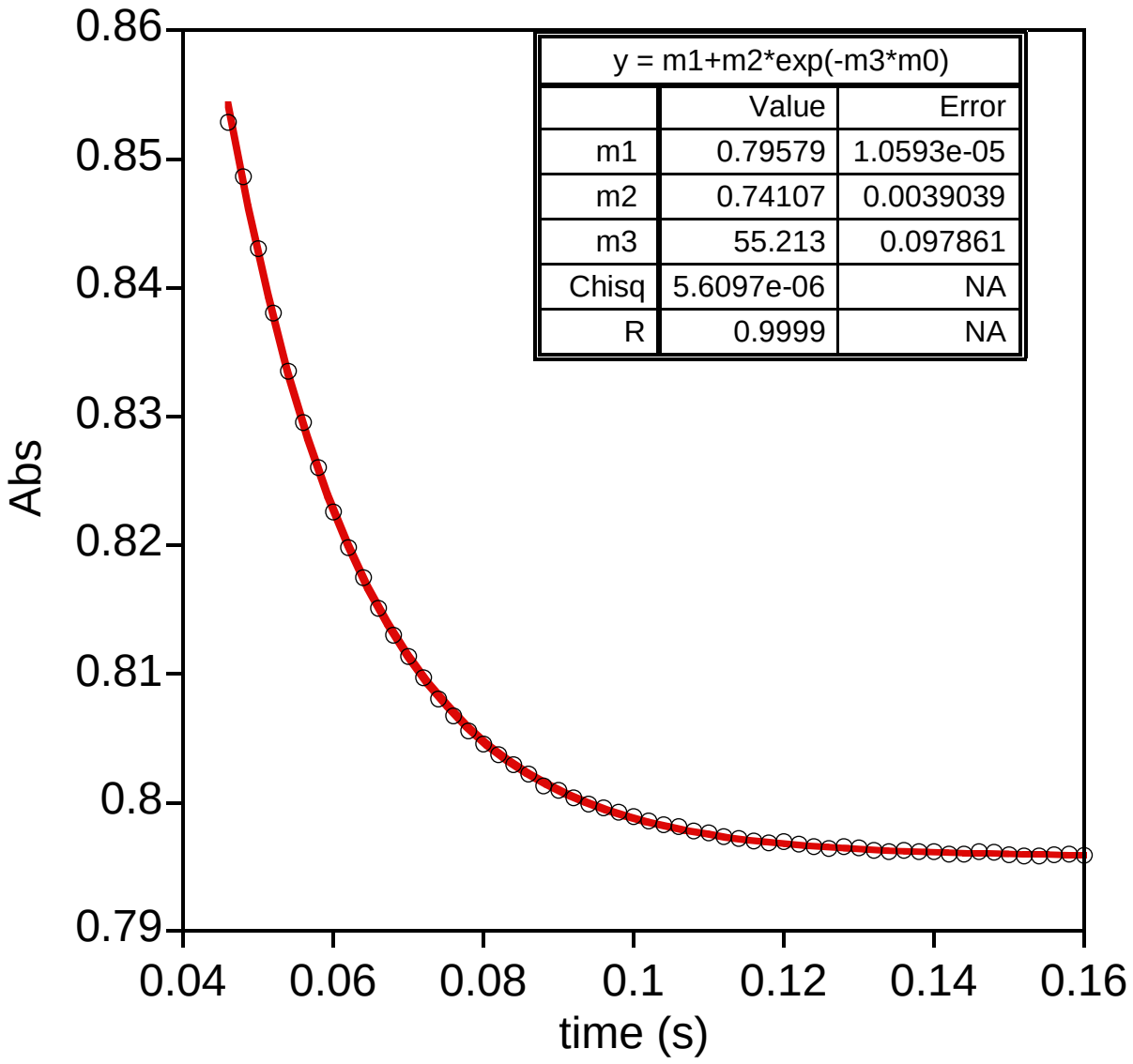

Figure S9. Observed absorbance decrease at 412 nm for the reaction of chlorinated *E. coli* (6 μM, based upon the HOCl used) with SCN^- (2.5 mM) for 12 minutes, followed by reaction with TNB (58.66 μM) at pH 7.4 and I = 1.0 M. A first-order fit (red) and 50% of the data (black circles) are illustrated.