12/5/24, 5:37 PM endpoint-fit

```
In [1]: import numpy as np
        from scipy.integrate import odeint
        from scipy.optimize import curve_fit
        from scipy.optimize import differential evolution
        %matplotlib inline
        import matplotlib.pyplot as plt
        from matplotlib.backends.backend_pdf import PdfPages
        import pandas as pd
In [2]: from endpoint_maker import sqres
        from endpoint maker import func
        from endpoint maker import t
        from endpoint maker import new
        from endpoint maker import lightdata
        from endpoint_maker import rawdata
In [3]: if name == ' main ':
            def initparams():
                \#bounds = ([0.00001,10000],[0,4],[0.00001,1000],[0.00001,1000],[0.00001,100
                bounds = ([0.00001,1000],[0.00001,1000],[0.00001,10000],[0.00001,10000])
                result = differential evolution(sqres,bounds,maxiter=100,popsize=20,polish=
                return result
In [4]: initialp = initparams()
        print(initialp)
        message: Maximum number of iterations has been exceeded.
        success: False
            fun: 0.17845065007023944
              x: [ 9.840e+02 6.203e-01 1.043e-05 9.624e+03]
            nit: 100
           nfev: 8080
In [5]: #def tester(t,Kd,n,d2,k2,k3,i):
        def tester(t,d2,k2,k3,k7,i):
            inivalues = [1,0,0,0,0,0,0]
            arrayvalues = np.asarray([])
            #for i in range(len(lightdata[:,0])):
            def I(t):
                tindex = t/5
                if tindex > 12241:
                    tindex = 12240
                return lightdata[i][int(tindex)]
            \#def\ odes(z,t,Kd,n,d2,k2,k3):
            def odes(z,t,d2,k2,k3,k7):
                Pu, Pb, Pa, mRNA, mCherry1, mCherry2, mCherry3 = z
                d1 = 0.019905
                k1 = 0.08299
                Kd = 90.41
                n = 0.964487
                #d2= 486.67
```

12/5/24, 5:37 PM endpoint-fit

```
\#k2 = 6.597
    #k3= 0.0539
    d3 = 0.000077
    k4 = 1.25
    d4 = 0.000031
    k5 = 0.00283
    k6 = 0.00283
    Pu = z[0]
    Pb = z[1]
    Pa = z[2]
    mRNA = z[3]
    mCherry1 = z[4]
    mCherry2 = z[5]
    mCherry3 = z[6]
    dPudt = d1*Pb - k1*I(t)*Pu + k7*I(t)**n/(Kd**n+I(t)**n)*Pa
    dPbdt = k1*I(t)*Pu - k2*Pb - d1*Pb + d2*Pa
    dPadt = k2*Pb - d2*Pa - k7*I(t)**n/(Kd**n+I(t)**n)*Pa
    dmRNAdt = k3*Pa - d3*mRNA
    dmCherry1dt = k4*mRNA-(d4 + k5)*mCherry1
    dmCherry2dt = k5*mCherry1-(d4+k6)*mCherry2
    dmCherry3dt = k6*mCherry2 - d4*mCherry3
    return [dPudt,dPbdt,dPadt,dmRNAdt,dmCherry1dt,dmCherry2dt,dmCherry3dt]
\#solver = odeint(odes,inivalues,t,args = (Kd,n,d2,k2,k3),hmax=0.1)
solver = odeint(odes,inivalues,t,args = (d2,k2,k3,k7),hmax=0.1)
mCherryout = solver[:,6]
#mCherryout = mCherryout[0:24480:240]
return mCherryout
```

```
In [6]: print(initialp.x)
```

[9.84019831e+02 6.20279494e-01 1.04268611e-05 9.62380222e+03]

12/5/24, 5:37 PM endpoint-fit

C:\Users\Leandra\anaconda3\Lib\site-packages\scipy\integrate_odepack_py.py:248: ODE
intWarning: Excess work done on this call (perhaps wrong Dfun type). Run with full_o
utput = 1 to get quantitative information.
 warnings.warn(warning_msg, ODEintWarning)
d2= 1002.8572605746836 k2= 0.7423885493341206 k3= 9.221127849160637e-06 k7= 61715.38
2923276775

```
In [8]: import sys
        import numpy
        \#params = [1,1,1,1,1,1,1]
        params = [1,1,1,1]
        numpy.set_printoptions(threshold=10)
        \#model1 = np.asarray(func(t,Kd,n,d2,k2,k3))
        model1 = np.asarray(func(t,d2,k2,k3,k7))
        print(len(model1))
        #print(model1)
        \#a,b,c,d,e,f,g = params
        a,b,c,d = params
        ydata = np.asarray(new)
        print(len(ydata))
        ssr = np.sum((ydata-model1)**2)
        #ssr2 = np.sum((ydata-model2)**2)
        sst = np.sum((ydata - np.mean(ydata))**2)
        R2 = 1 - ssr/sst
        \#R2_2 = 1 - ssr2/sst
        print('R2 is: ', R2)
        #print(R2_2)
```

102 102 R2 is: 0.8374633104557399

```
In [9]: pp = PdfPages('multipage.pdf')
        ydata = np.asarray(new)
         \#condition = [1,2,3,4,5,6,7,8,9]
        for i in range(2):
             \#model = tester(t, Kd, n, d2, k2, k3, i)
            model = tester(t,d2,k2,k3,k7,i)
            #print(model)
            \#a,b,c,d,e,f,g= params
            a,b,c,d= params
            plt.plot(t,model,'.', label = 'model')
            #print(model)
            \#t = np.linspace(0,34800, num=6961)
            #raw = rawdata[0:13920:240]
            plt.plot(t,raw[i],'.',label = 'data')
            #print(rawdata[i])
            plt.legend()
            pp.savefig()
```

12/5/24, 5:37 PM endpoint-fit

```
plt.show()
pp.close
```

```
NameError
                                          Traceback (most recent call last)
Cell In[9], line 17
     13 plt.plot(t,model,'.', label = 'model')
     14 #print(model)
     15 #t = np.linspace(0,34800, num=6961)
     16 #raw = rawdata[0:13920:240]
---> 17 plt.plot(t,raw[i],'.',label = 'data')
     18 #print(rawdata[i])
     19 plt.legend()
```

NameError: name 'raw' is not defined

