

> **restart:**

Define Etotal and obtain in terms of equilibrium coefficient, E and M only

> **eqn1:={Etotal=E+ME};**

$$eqn1 := \{Etotal = E + ME\}$$

> **eqn2:=algsubs(ME=BME*M*E, eqn1);**

$$eqn2 := \{Etotal = E + BME M E\}$$

Now obtain E as function of Etotal

> **solve(eqn2,E);**

$$\left\{ E = \frac{Etotal}{1 + BME M} \right\}$$

Now, work towards getting M in terms of equilibrium coefficient and E, which will allow us to solve E and M

> **eqn3:= {Mtotal=M+ME};**

$$eqn3 := \{Mtotal = M + ME\}$$

> **eqn4:= algsubs(ME=BME*M*E, eqn3);**

$$eqn4 := \{Mtotal = M + BME M E\}$$

Substitute the expression for E found earlier, giving Mtotal in terms of equilibrium coefficients and M only

> **eqn5:= algsubs(E = Etotal/(1+BME*M), eqn4);**

$$eqn5 := \left\{ Mtotal = \frac{M (1 + BME M + BME Etotal)}{1 + BME M} \right\}$$

> **Msol := solve(Mtotal = $\frac{M (1 + BME M + BME Etotal)}{1 + BME M}$,
 M);**

$$Msol := -\frac{1}{2} \frac{1}{BME} \left(-Mtotal BME + 1 + BME Etotal \right. \\
 - \left(Mtotal^2 BME^2 + 2 Mtotal BME \right. \\
 \left. - 2 Mtotal BME^2 Etotal + 1 + 2 BME Etotal + BME^2 Etotal^2 \right)^{1/2}, \\
 -\frac{1}{2} \frac{1}{BME} \left(-Mtotal BME + 1 + BME Etotal \right. \\
 + \left(Mtotal^2 BME^2 + 2 Mtotal BME \right. \\
 \left. - 2 Mtotal BME^2 Etotal + 1 + 2 BME Etotal + BME^2 Etotal^2 \right)^{1/2} \left. \right)$$

Obviously the first solution was the important one. Now, we can obtain E

> **Esol:=Etotal/(1+BME*Msol[1]);**

$$Esol := Etotal / \left(\frac{1}{2} + \frac{1}{2} Mtotal BME - \frac{1}{2} BME Etotal \right. \\
 + \frac{1}{2} \left(Mtotal^2 BME^2 + 2 Mtotal BME \right. \\
 \left. - 2 Mtotal BME^2 Etotal + 1 + 2 BME Etotal + BME^2 Etotal^2 \right)^{1/2} \left. \right)$$

Having M and E we can obtain ME

> **MEsol := BME * Msol[1] * Esol;**

$$\begin{aligned}
 MEsol := & -\frac{1}{2} \left((-Mtotal \ BME + 1 + BME \ Etotal \right. \\
 & - (Mtotal^2 \ BME^2 + 2 \ Mtotal \ BME \\
 & - 2 \ Mtotal \ BME^2 \ Etotal + 1 + 2 \ BME \ Etotal + BME^2 \ Etotal^2) \\
 & \left. ^{1/2} \right) \left/ \left(\frac{1}{2} + \frac{1}{2} \ Mtotal \ BME - \frac{1}{2} \ BME \ Etotal \right. \right. \\
 & + \frac{1}{2} (Mtotal^2 \ BME^2 + 2 \ Mtotal \ BME \\
 & \left. \left. - 2 \ Mtotal \ BME^2 \ Etotal + 1 + 2 \ BME \ Etotal + BME^2 \ Etotal^2) \right. \right. \\
 & \left. \left. ^{1/2} \right) \right.
 \end{aligned}$$

Now we can substitute the concentrations of M and ME into the expression for the observed fluorescence in terms of molar emission coefficients for M and ME

> **eqn6 := IM * Msol[1] + IME * MEsol;**

$$\begin{aligned}
 eqn6 := & -\frac{1}{2} \frac{1}{BME} \left(IM \left(-Mtotal \ BME + 1 + BME \ Etotal \right. \right. \\
 & - (Mtotal^2 \ BME^2 + 2 \ Mtotal \ BME \\
 & - 2 \ Mtotal \ BME^2 \ Etotal + 1 + 2 \ BME \ Etotal + BME^2 \ Etotal^2) \\
 & \left. \left. ^{1/2} \right) - \frac{1}{2} \left(IME \left(-Mtotal \ BME + 1 + BME \ Etotal \right. \right. \right. \\
 & - (Mtotal^2 \ BME^2 + 2 \ Mtotal \ BME \\
 & - 2 \ Mtotal \ BME^2 \ Etotal + 1 + 2 \ BME \ Etotal + BME^2 \ Etotal^2) \\
 & \left. \left. ^{1/2} \right) \right) \left/ \left(\frac{1}{2} + \frac{1}{2} \ Mtotal \ BME - \frac{1}{2} \ BME \ Etotal \right. \right. \\
 & + \frac{1}{2} (Mtotal^2 \ BME^2 + 2 \ Mtotal \ BME \\
 & \left. \left. - 2 \ Mtotal \ BME^2 \ Etotal + 1 + 2 \ BME \ Etotal + BME^2 \ Etotal^2) \right. \right. \\
 & \left. \left. ^{1/2} \right) \right.
 \end{aligned}$$

Now substitute some trial values for SCC

> **IntensitySCC := subs (BME = 1000000, IM = $\frac{0.838}{Mtotal}$, IME = $\frac{2}{Mtotal}$, Mtotal = 0.00005, eqn6);**

$$\begin{aligned} \text{IntensitySCC} := & 0.4106200000 - 8380.000000 E_{\text{total}} \\ & + 0.008380000000 \\ & \sqrt{2601.000000 - 9.8000000010^7 E_{\text{total}} + 100000000000 E_{\text{total}}^2} \\ & - (20000.00000 (-49.00000 + 1000000 E_{\text{total}} \\ & - \\ & (2601.000000 - 9.8000000010^7 E_{\text{total}} \\ & + 100000000000 E_{\text{total}}^2)^{1/2}) E_{\text{total}} \Big/ \left(25.500000000 \right. \\ & - 500000 E_{\text{total}} \\ & + \frac{1}{2} \\ & \left. (2601.000000 - 9.8000000010^7 E_{\text{total}} \right. \\ & \left. + 100000000000 E_{\text{total}}^2)^{1/2} \right) \end{aligned}$$

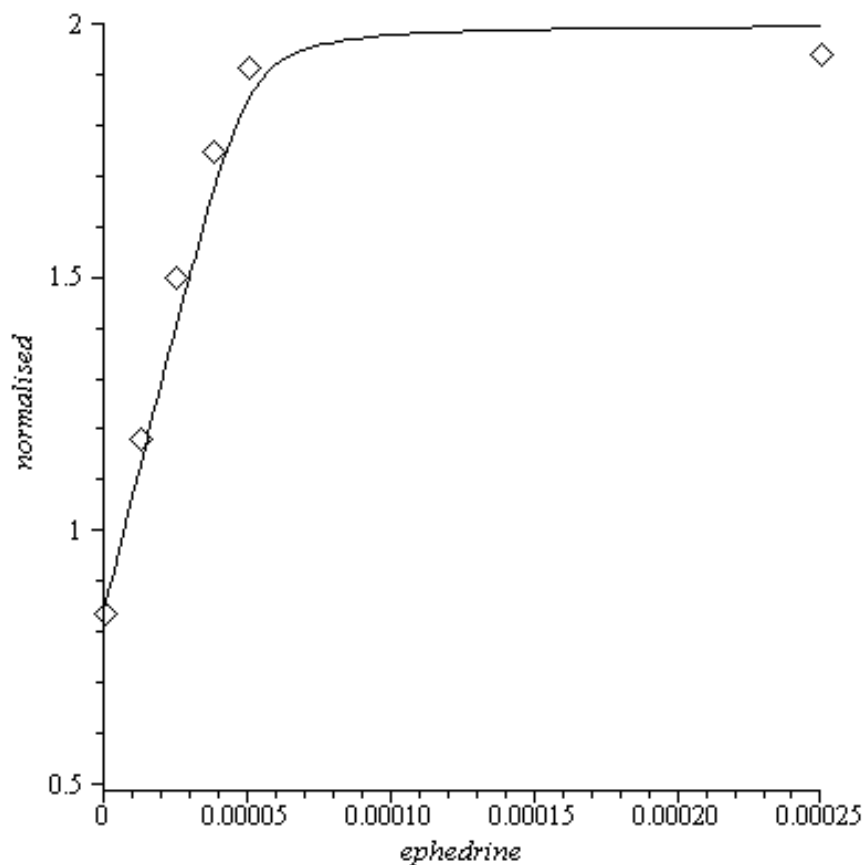
this command is needed for Maple to use its full graphing capability

```
> with(plots);
```

```
[animate, animate3d, animatecurve, arrow, changecoords ,  
complexplot, complexplot3d, conformal, conformal3d ,  
contourplot, contourplot3d, coordplot, coordplot3d, densityplot,  
display, dualaxisplot, fieldplot, fieldplot3d, gradplot,  
gradplot3d, graphplot3d, implicitplot, implicitplot3d, inequal,  
interactive, interactiveparams, intersectplot, listcontplot,  
listcontplot3d, listdensityplot, listplot, listplot3d, loglogplot,  
logplot, matrixplot, multiple, odeplot, pareto, plotcompare,  
pointplot, pointplot3d, polarplot, polygonplot, polygonplot3d ,  
polyhedra_supported , polyhedraplot, rootlocus, semilogplot,  
setcolors, setoptions, setoptions3d, spacecurve ,  
sparsematrixplot, surfdata, textplot, textplot3d, tubeplot ]
```

The data for SCC emission at 510 nm

```
> dataSCC :=  
{[0,0.838247],[0.0000125,1.185894],[0.000025,1.50246  
],[0.0000375,1.749829],[0.00005,1.916836],[0.00025,1.944795  
]}:  
> pntplotSCC :=  
pointplot(dataSCC,symbol=diamond,symbolsize=20);  
pntplotSCC := PLOT(...)  
> intensityplotSCC :=  
plot(IntensitySCC,Etotal=0..0.00025,color=black):  
display([pntplotSCC,intensityplotSCC],view=[0..0.00025,0.5.  
.2],labels=[ephedrine,  
normalised],labeldirections=[horizontal, vertical]);
```



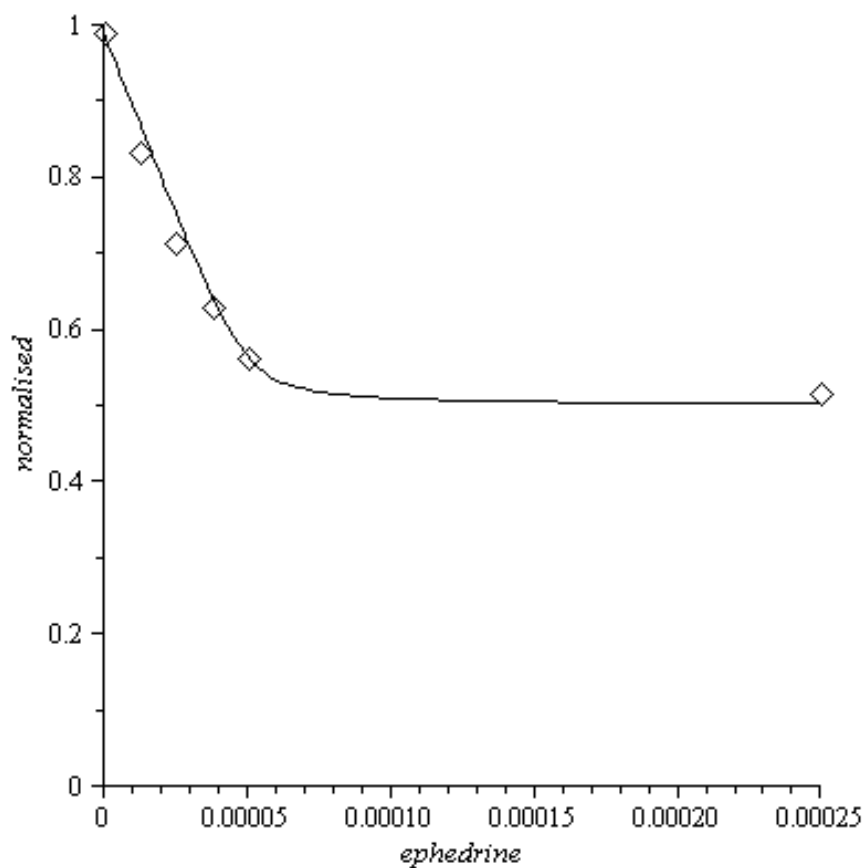
Now some trial values for VCC

```
> IntensityVCC := subs(BME = 1000000, IM = .991/Mtotal, IME
= 0.5/Mtotal, Mtotal = 0.5e-4, eqn6);
```

$$\begin{aligned}
 \text{IntensityVCC} := & 0.4855900000 - 9910.000000Etotal \\
 & + 0.009910000000 \\
 & \frac{\sqrt{2601.000000 - 9.8000000010^7 Etotal + 1000000000000Etotal^2}}{25.50000000} \\
 & - \left(5000.000000(-49.00000 + 1000000Etotal) \right. \\
 & \left. - \left(2601.000000 - 9.8000000010^7 Etotal \right. \right. \\
 & \left. \left. + 1000000000000Etotal^2 \right)^{1/2} \right) Etotal \\
 & - 500000Etotal \\
 & + \frac{1}{2} \\
 & \left(2601.000000 - 9.8000000010^7 Etotal \right. \\
 & \left. + 1000000000000Etotal^2 \right)^{1/2}
 \end{aligned}$$

and the data for VCC at 510 nm

```
> dataVCC := {[0, 0.990993], [0.0000125, 0.834232], [0.000025, 0.7139],  
  ], [0.0000375, 0.631177], [0.00005, 0.565339], [0.00025, 0.517887]} :  
  
> pntplotVCC :=  
pointplot(dataVCC, symbol=diamond, symbolsize=20);  
      pntplotVCC := PLOT(...)  
  
> intensityplotVCC:=  
plot(IntensityVCC, Etotal=0..0.00025, color=black):  
display([pntplotVCC, intensityplotVCC], view=[0..0.00025, 0..1  
], labels=[ephedrine,  
normalised], labeldirections=[horizontal, vertical]);
```



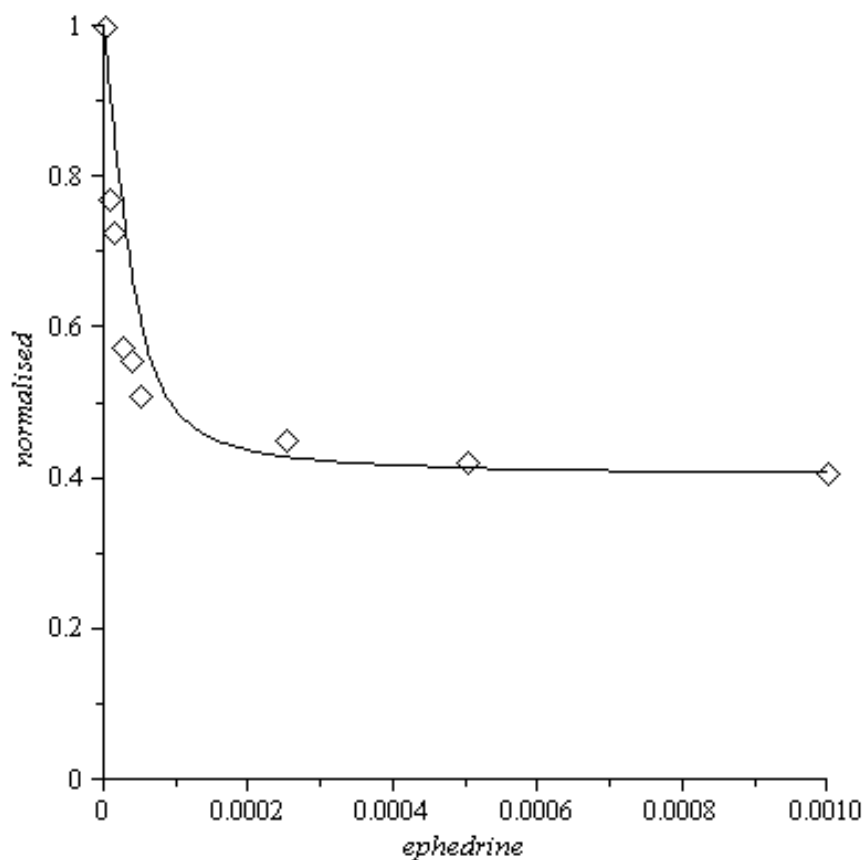
Now some trial values for PV

```
> IntensityPV := subs(BME = 100000, IM = 1/Mtotal, IME =  
0.4/Mtotal, Mtotal = 0.5e-4, eqn6);
```

$$\begin{aligned} \text{IntensityPV} := & 0.4000000000 - 10000.00000Etotal \\ & + 0.1000000000 \\ & \frac{\sqrt{36.00000000 - 8.0000000010^5 Etotal + 10000000000Etotal^2} - (4000.000000(-4.00000 + 100000Etotal} \\ & - \sqrt{36.00000000 - 8.0000000010^5 Etotal + 10000000000Etotal^2})}{Etotal} \Bigg/ \left(3.000000000 - 50000Etotal \right. \\ & \left. + \frac{1}{2} \sqrt{36.00000000 - 8.0000000010^5 Etotal + 10000000000Etotal^2} \right) \end{aligned}$$

and the data for PV at 454 nm

```
> dataPV := {[0, 1], [0.00000625 0.772236], [0.0000125 0.72846],  
             [0.000025 0.573828], [0.0000375 0.558383], [0.00005 0.50982],  
             [0.00025 0.452838], [0.0005 0.421438], [0.001, 0.408197]} :  
  
> pntplotPV :=  
pointplot(dataPV, symbol=diamond, symbolsize=20);  
           pntplotPV := PLOT(...)  
  
> intensityplotPV :=  
plot(IntensityPV, Etotal=0..0.001, color=black):  
display([pntplotPV, intensityplotPV], view=[0..0.001, 0..1], la  
bels=[ephedrine, normalised], labeldirections=[horizontal,  
vertical]);
```



Now some trial values for PS

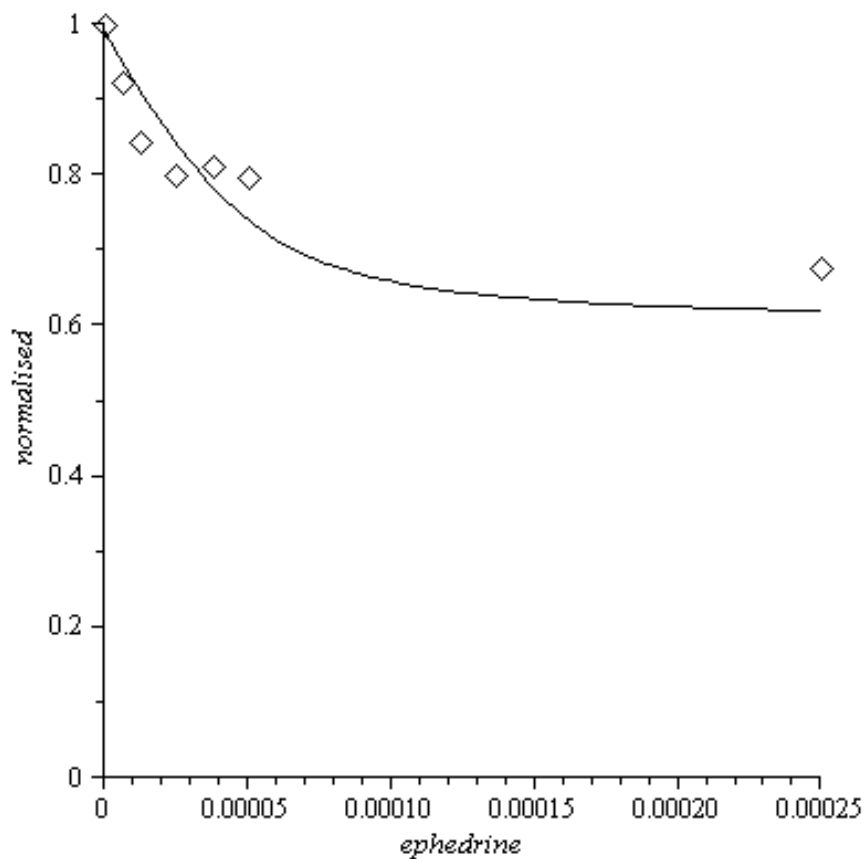
```
> IntensityPS := subs(BME = 100000, IM = .991/Mtotal, IME = 0.6/Mtotal, Mtotal = 0.5e-4, eqn6);
```

$$\begin{aligned}
 \text{IntensityPS} := & 0.3964000000 - 9910.000000Etotal \\
 & + 0.0991000000 \\
 & \sqrt{36.00000000 - 8.000000010^5 Etotal + 10000000000Etotal^2} \\
 & - (6000.000000(-4.00000 + 100000Etotal \\
 & - \\
 & \sqrt{36.00000000 - 8.000000010^5 Etotal + 10000000000Etotal^2}) \\
 & Etotal) / \left(3.000000000 - 50000Etotal \right. \\
 & \left. + \frac{1}{2} \sqrt{36.00000000 - 8.000000010^5 Etotal + 10000000000Etotal^2} \right)
 \end{aligned}$$

and the data for PS at 510 nm

```
> dataPS := {[0, 1], [0.00000625 0.923817], [0.0000125 0.844778],
    [0.000025 0.801754], [0.0000375 0.813593], [0.00005 0.796886],
    [0.00025 0.677061], [0.0005 0.633561], [0.001, 0.621755]} :
```

```
> pntplotPS :=  
pointplot(dataPS,symbol=diamond,symbolsize=20);  
      pntplotPS :=PLOT(...)  
> intensityplotPS:=  
plot(IntensityPS,Ettotal=0..0.00025,color=black):  
display([pntplotPS,intensityplotPS],view=[0..0.00025,0..1],  
labels=[ephedrine, normalised],labeldirections=[horizontal,  
vertical]);
```



```
> ?  
> ?
```