

Peptide Supply Fit For Both

Ruth Eccleston

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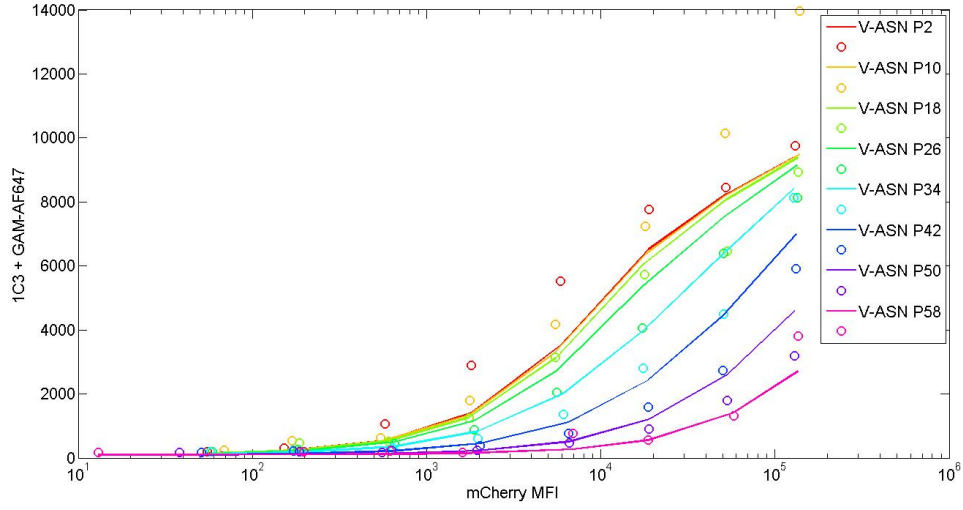
1 150422 ASN SSL IFN none and IFN +

1.1 Attempt 2

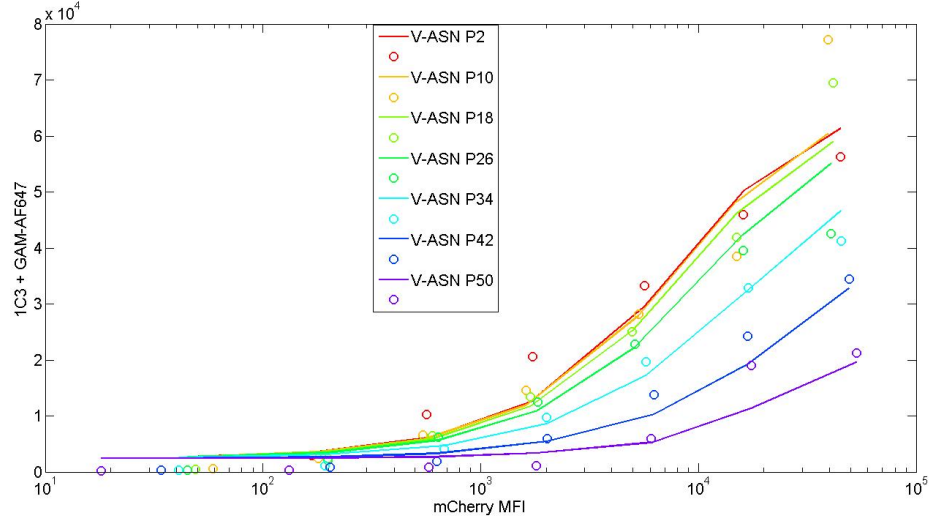
Parameters	
Time to Initialise	5 hrs
Time for Simulation	24 hrs
Self Peptide Supply	0 molecules/s
bP_T	$3.177334 \times 10^{-11} / \text{molecules/s}$
bP_C	$3.177334 \times 10^{-11} / \text{molecules/s}$

- Fitting Method 1: Fit for sf1 and sf2 for both $+/-$ IFN (same sf1 and sf2 for both) to fit for supply, and also fit for gM1 and gM2, for - IFN and + IFN respectively (where $gT = 10 * gM$), then scale output cell surface data using polyfit ie $p1 * MeP1 + p2$ to get best fit to data (different polyfit for $+/-$ IFN).
- $err = err_{none} + err_{ifn}$
- $sf0 = [1, 1, 105.5, 10000.5]$

Best Fit Scale Factors	
sf1	0.8008
sf2	4.3651
gM1	6.6763
gM2	102.7993
$p1_{none}$	0.0542
$p2_{none}$	100.6828
$p1_{ifn}$	0.0130
$p2_{ifn}$	2.4127×10^3
err	$3.9562 \times 10^{+04}$



(a)



(b)

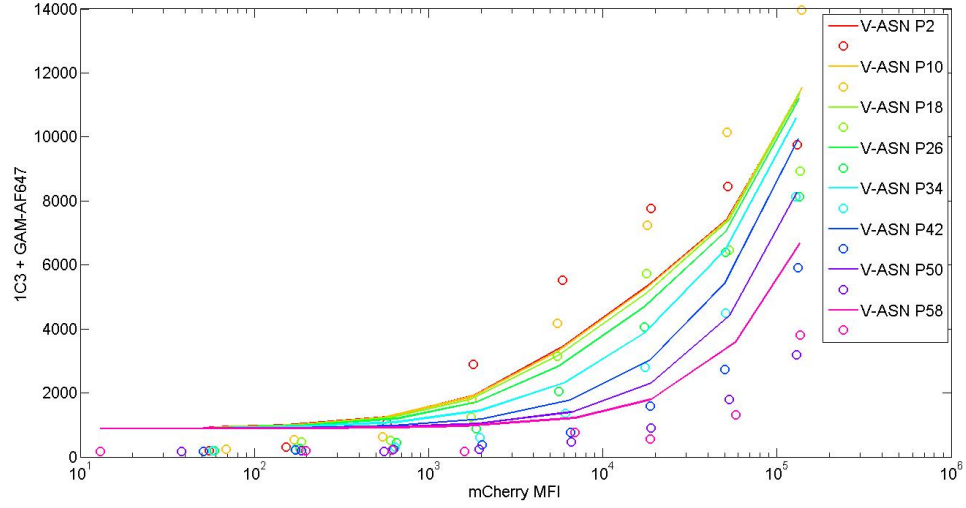
Figure 1: $t_i = 5hrs$, $t_s = 24hrs$, $sf1 = 0.8008$, $sf2 = 4.3651$, $gM1 = 6.6763$, $gM2 = 102.7993$

1.2 Attempt 3

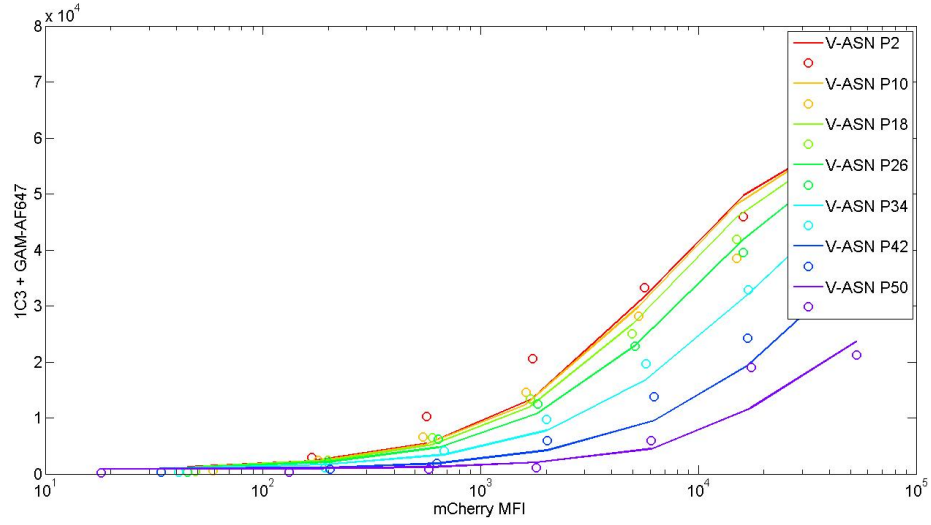
Parameters	
Time to Initialise	10 hrs
Time for Simulation	5 hrs
Self Peptide Supply	$0molecules/s$
bP_T	$3.177334 \times 10^{-11}/molecules/s$
bP_C	$3.177334 \times 10^{-11}/molecules/s$

- Fitting Method 2: Fit for $sf1$ and $sf2$ for both $+/-$ IFN (same $sf1$ and $sf2$ for both) to fit for supply, and also fit for $gM1$ and $gM2$, for $-$ IFN and $+$ IFN respectively (where $gT = 10 * gM$), then scale output cell surface data using polyfit ie $p1 * MeP1 + p2$ to get best fit to data, using the same polyfit for polyfit for $+/-$ IFN.
- $sf0 = [1, 1, 105.5, 10000.5]$

Best Fit Scale Factors	
sf1	0.2210
sf2	1.0517
gM1	0.4256
gM2	1.6586
$p1_{both}$	3.1581
$p2_{both}$	885.7649
err	$3.3076 \times 10^{+04}$



(a)



(b)

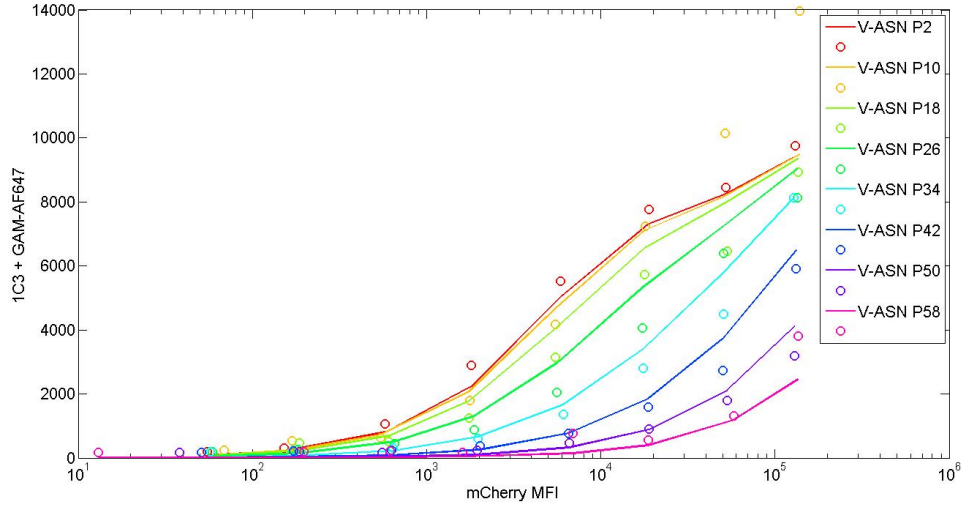
Figure 2: $t_i = 10hrs$, $t_s = 5hrs$, $sf1 = 0.221$, $sf2 = 1.0517$, $gM1 = 0.4256$, $gM2 = 1.6586$

1.3 Attempt 4

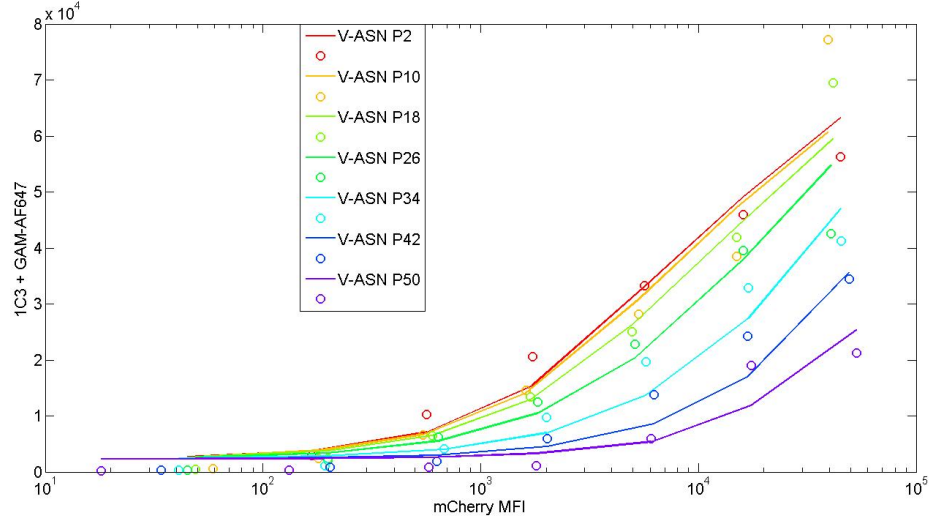
Parameters	
Time to Initialise	24 hrs
Time for Simulation	5 days
Self Peptide Supply	0 molecules/s
bP_T	$3.177334 \times 10^{-11} / \text{molecules/s}$
bP_C	$3.177334 \times 10^{-11} / \text{molecules/s}$

- Fitting Method 1: Fit for sf1 and sf2 for both $+/-$ IFN (same sf1 and sf2 for both) to fit for supply, and also fit for gM1 and gM2, for - IFN and + IFN respectively (where $gT = 10 * gM$), then scale output cell surface data using polyfit ie $p1 * MeP1 + p2$ to get best fit to data (different polyfit for $+/-$ IFN).
- $err = err_{none} + err_{ifn}$
- $sf0 = [1, 1, 105.5, 10000.5]$

Best Fit Scale Factors	
sf1	0.2528
sf2	2.0310
gM1	2.6634
gM2	0.7632
$p1_{none}$	0.1906
$p2_{none}$	2.9975
$p1_{ifn}$	11.60
$p2_{ifn}$	2.3058×10^3
err	$3.8597 \times 10^{+04}$



(a)



(b)

Figure 3: $t_i = 24hrs$, $t_s = 5days$, $sf1 = 0.2528$, $sf2 = 2.0310$, $gM1 = 2.6634$, $gM2 = 0.7632$

1.4 Attempt 5

Parameters	
Time to Initialise	24 hrs
Time for Simulation	10 hrs
Self Peptide Supply	0 molecules/s
bP_T	$3.177334 \times 10^{-11} / \text{molecules/s}$
bP_C	$3.177334 \times 10^{-11} / \text{molecules/s}$

- Fitting Method 1: Fit for $sf1$ and $sf2$ for both $+/-$ IFN (same $sf1$ and $sf2$ for both) to fit for supply, and also fit for $gM1$ and $gM2$, for $-$ IFN and $+$ IFN respectively (where $gT = 10 * gM$), then scale output cell surface data using polyfit ie $p1 * MeP1 + p2$ to get best fit to data (different polyfit for $+/-$ IFN).
- $err = err_{none} + err_{ifn}$

- $sf0 = [1, 1, 105.5, 10000.5]$

Best Fit Scale Factors	
sf1	1.2203
sf2	5.6610
gM1	2.0098
gM2	39.8554
$p1_{none}$	0.2275
$p2_{none}$	163.3102
$p1_{ifn}$	0.0240
$p2_{ifn}$	2.5125×10^3
err	$4.0792 \times 10^{+04}$

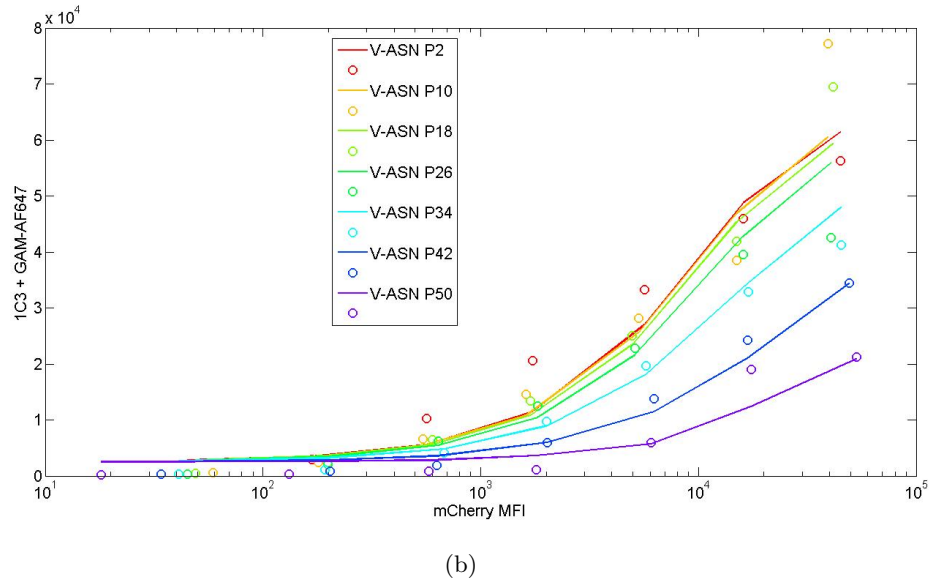
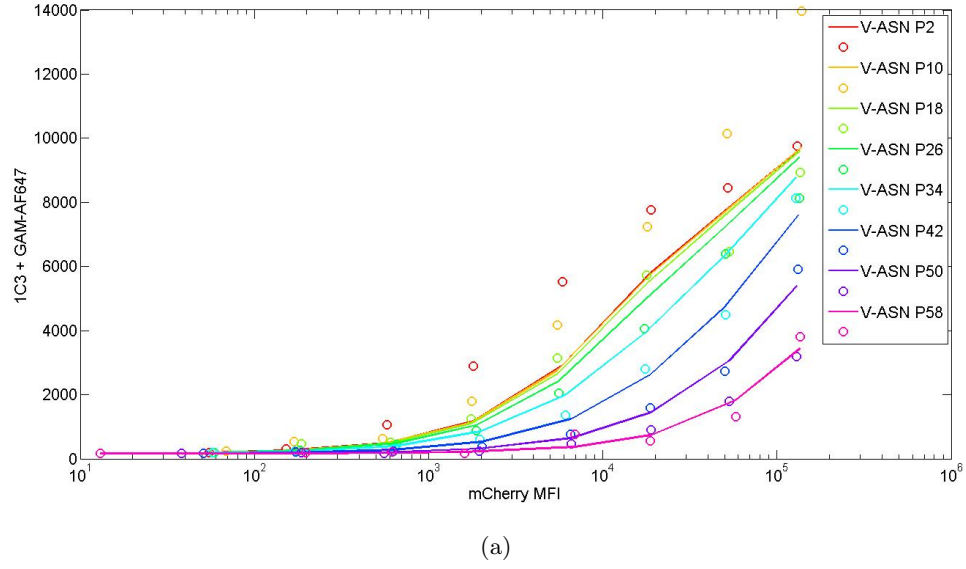


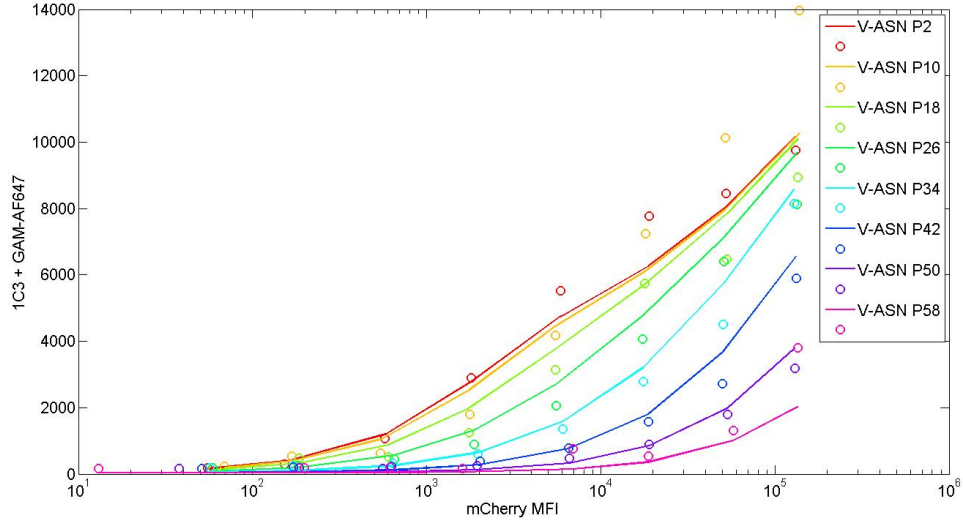
Figure 4: Best fit to the data for a) Fitting method 1, b) Fitting method 2, where the best fit scale factors are given in tables 2 and 3 respectively

1.5 Attempt 6

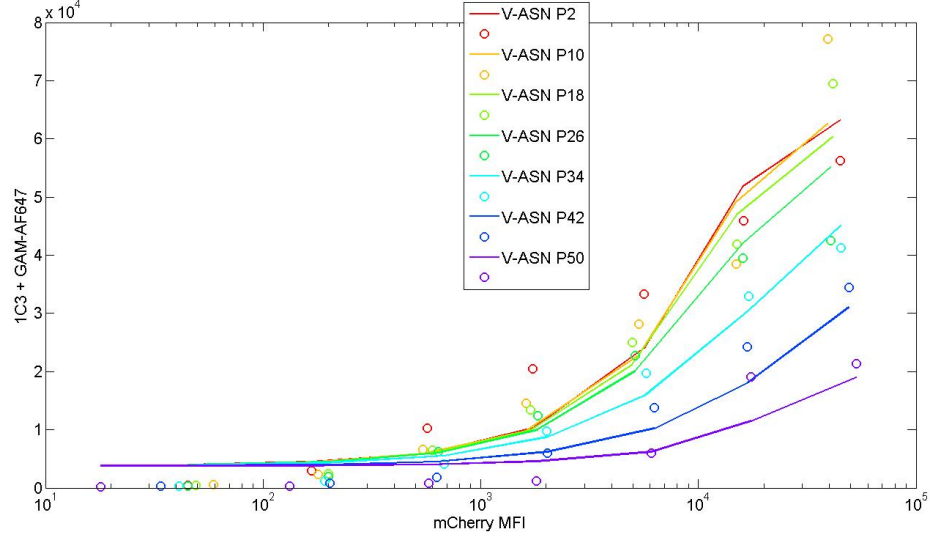
Parameters	
Time to Initialise	0 hrs
Time for Simulation	24 hrs
Self Peptide Supply	0 molecules/s
bP_T	$3.177334 \times 10^{-11} / \text{molecules/s}$
bP_C	$3.177334 \times 10^{-11} / \text{molecules/s}$

- Fitting Method 1: Fit for sf1 and sf2 for both $+/-$ IFN (same sf1 and sf2 for both) to fit for supply, and also fit for gM1 and gM2, for - IFN and + IFN respectively (where $gT = 10 * gM$), then scale output cell surface data using polyfit ie $p1 * MeP1 + p2$ to get best fit to data (different polyfit for $+/-$ IFN).
- $err = err_{none} + err_{ifn}$
- $sf0 = [10, 20, 100, 1e6]$

Best Fit Scale Factors	
sf1	4.6506
sf2	28.6018
gM1	4.9436
gM2	$6.2284 \times 10^{+04}$
$p1_{none}$	0.0628
$p2_{none}$	37.8125
$p1_{ifn}$	2.0892×10^{-05}
$p2_{ifn}$	$3.7830e \times 10^3$
err	$4.2644 \times 10^{+04}$



(a)



(b)

Figure 5: $t_i = 0hrs$, $t_s = 24hrs$, $sf1 = 4.6506$, $sf2 = 28.6018$, $gM1 = 4.9436$, $gM2 = 6.2284 \times 10^{+04}$

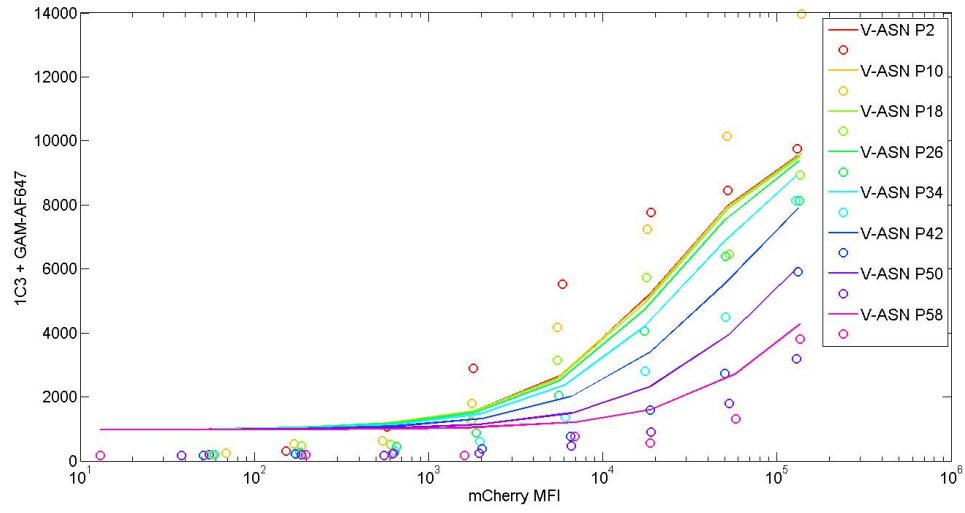
1.6 Attempt 7

Parameters	
Time to Initialise	1 hrs
Time for Simulation	10 days
Self Peptide Supply	$0molecules/s$
bP_T	$3.177334 \times 10^{-11}/molecules/s$
bP_C	$3.177334 \times 10^{-11}/molecules/s$

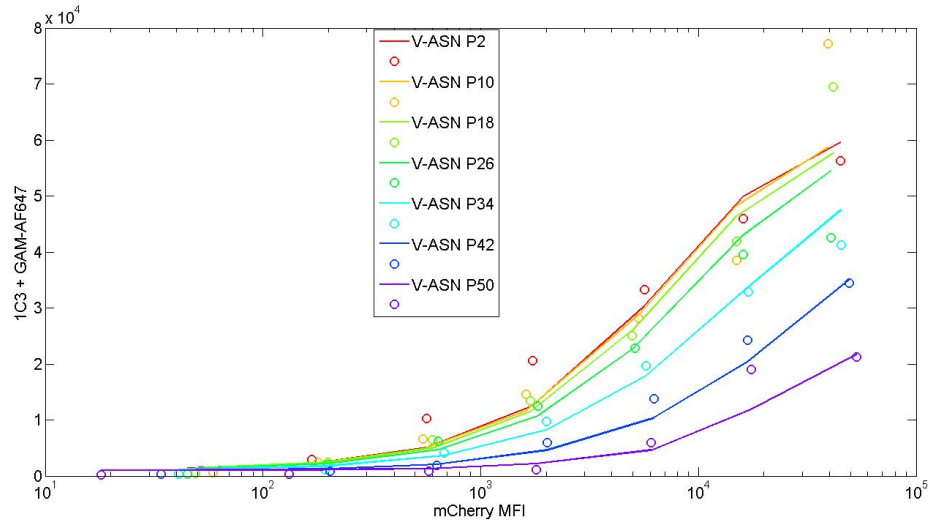
- Fitting Method 1: Fit for $sf1$ and $sf2$ - IFN and $sf1*upreg$, $sf2*upreg$ for + IFN to fit for supply, and also fit for $gM1$ for without IFN and $gM1*upreg$ for + IFN, (where $gT = 10 * gM$), then scale output cell surface data using polyfit ie $p1 * MeP1 + p2$ to get best fit to data (same polyfit for +/- IFN).

- $err = err_{none} + err_{ifn}$
- $sf0 = [10, 20, 100, 1e6]$

Best Fit Scale Factors	
sf1	0.0318
sf2	0.1372
gM1	1.6764
upreg	3.0594
$p1_{both}$	0.5060
$p2_{both}$	974.9214
err	$3.3416 \times 10^{+04}$



(a)



(b)

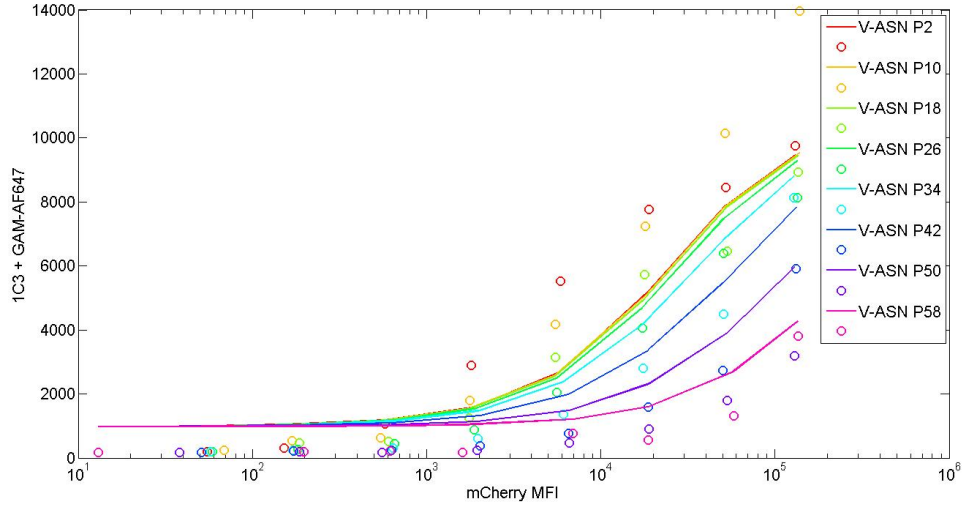
Figure 6: $t_i = 1hrs$, $t_s = 10days$, $sf1 = 0.0318$, $sf2 = 0.1372$, $gM1 = 1.6764$, $upreg = 3.0594$

1.7 Attempt 8

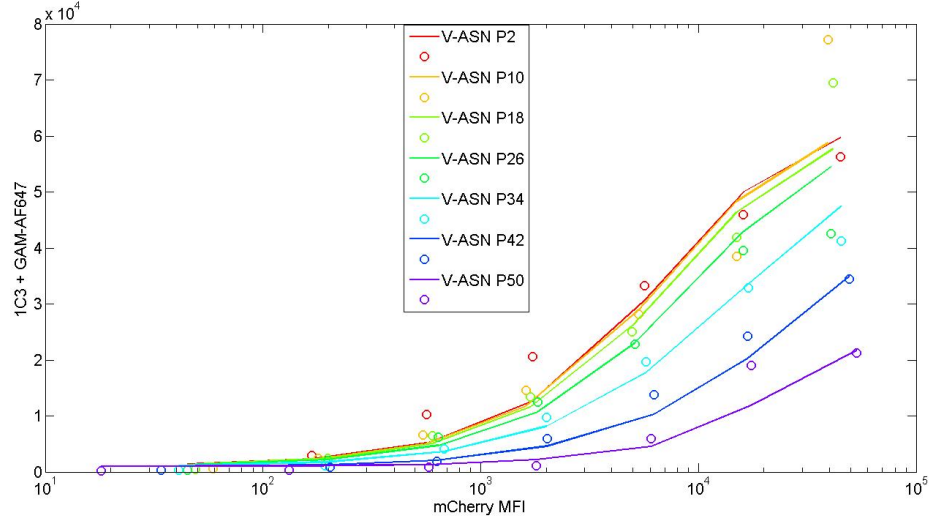
Parameters	
Time to Initialise	10 hrs
Time for Simulation	10 days
Self Peptide Supply	0 molecules/s
bP_T	$3.177334 \times 10^{-11} / \text{molecules/s}$
bP_C	$3.177334 \times 10^{-11} / \text{molecules/s}$

- Fitting Method 1: Fit for sf1 and sf2 - IFN and sf1*upreg, sf2*upreg for + IFN to fit for supply, and also fit for gM1 for without IFN and gM1*upreg for + IFN, (where $gT = 10 * gM$), then scale output cell surface data using polyfit ie $p1 * MeP1 + p2$ to get best fit to data (same polyfit for $+/-$ IFN).
- $err = err_{none} + err_{ifn}$
- $sf0 = [10, 20, 100, 1e6]$

Best Fit Scale Factors	
sf1	0.0317
sf2	0.1392
gM1	1.4937
upreg	3.0477
$p1_{both}$	0.6158
$p2_{both}$	981.6978
err	$3.3345 \times 10^{+04}$



(a)



(b)

Figure 7: $t_i = 0hrs$, $t_s = 24hrs$, $sf1 = 4.6506$, $sf2 = 28.6018$, $gM1 = 4.9436$, $gM2 = 6.2284 \times 10^{+04}$

- Attempt 7 vs attempt 8: Better fit in attempt 8 (lower err) for longer initialisation time but same simulation time. Rates quite similar for both. Upreg > 1 therefore $gM2 > gM1$ as required, and $sf1$ and $sf2 + IFN > sf1$ and $sf2 - IFN$ as would be expected.
- Using the same polyfit for both datasets means the fit to no IFN seems to suffer more than the fit to +IFN, most likely because the data values of + IFN are much larger than those for - IFN and so minimising the error from those data values will have a much larger influence on the overall error than minimising the error from the - IFN data set.
- Including the scale factor upreg for both $sf1$, $sf2$ and gM seems to improve the fit for -IFN compared to just for gM (compare attempt 3 for -IFN to attempts 7 and 8). Although the times used are not the same so perhaps a direct comparison not possible.
- Will try to include time in the fitting. If `fminsearch` not able to cope with 5 parameters may need to use `Filzbach`.