Peptide Supply Fit For Both

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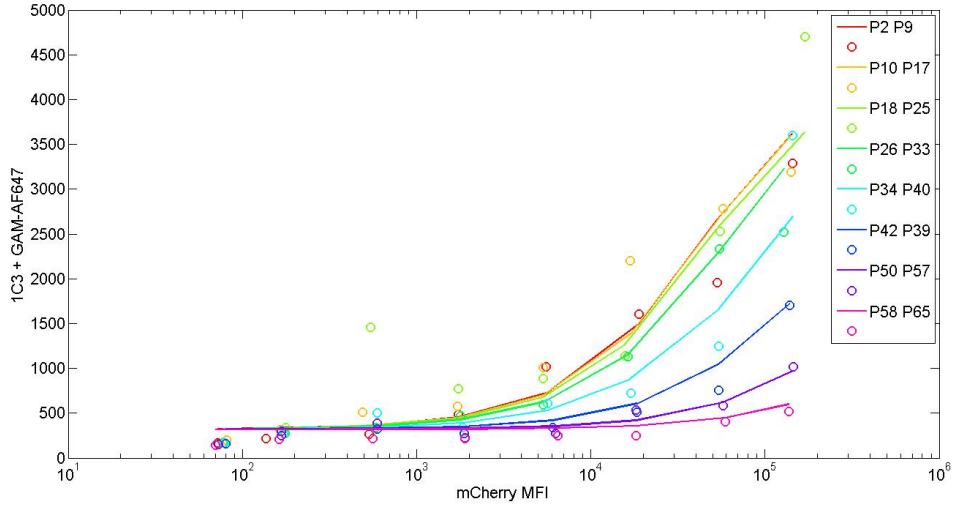# 1 150520-ASN-SSL-IFN-none

1.1 Attempt 1

Denise provided data for the cell surface abundance of the competitor peptide ASN as well as the target peptide SSL. However, the data does not appear to have been taken from the same experiment. The ASN cell surface data is provided along with the ASN cytoplasmic levels and the SSL cytoplasmic levels, however comparing these numbers to those given in the datasheet containing the SSL surface abundance, whilst they are generally similar to one another, they are not exactly the same. This difference becomes most significant for the larger concentrations of ASN or SSL in the cytoplasm. Therefore, to begin with I have simulated for the cell surface abundance of SSL using the SSL and ASN cytoplasmic levels for the first datasheet (with just the SSL surface abundance), and simulated for the ASN surface abundance separately (using the SSL and ASN cytoplasmic levels from the second datasheet with only the ASN surface levels). For both simulations I have required that the scale factors sf1 and sf2 for the cytoplasmic levels of SSL and ASN be the same when fitting to the data. For this initial attempt gM is set to the normal value of 105.5 and is not included in the fitting.

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

| Best Fit Scale Factors	
sf1	0.1897
sf2	4.5103
$p1_{MeSSL}$	0.0008
$p2_{MeSSL}$	317.4474
$p1_{MeASN}$	1.2361×10^{-05}
$p2_{MeASN}$	152.1105
err	$2.8080 \times 10^{+03}$
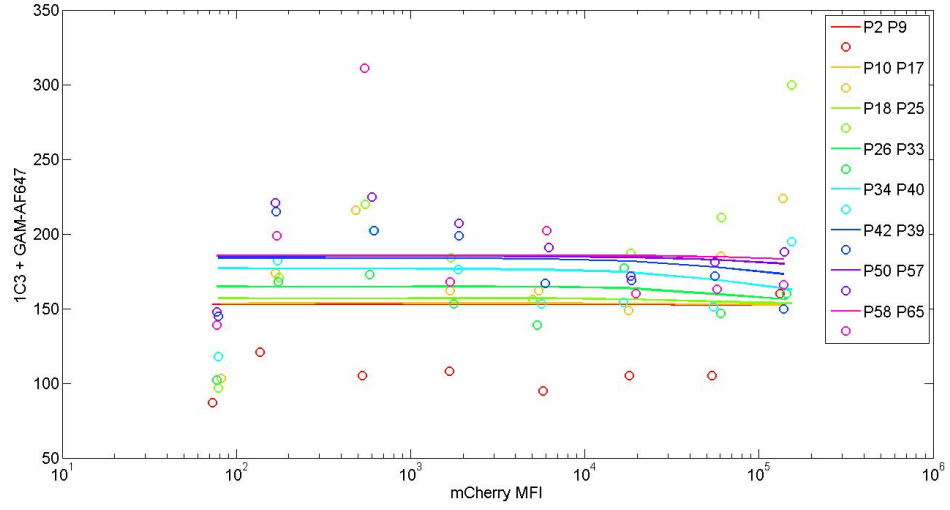
(a)

(b)

Figure 1

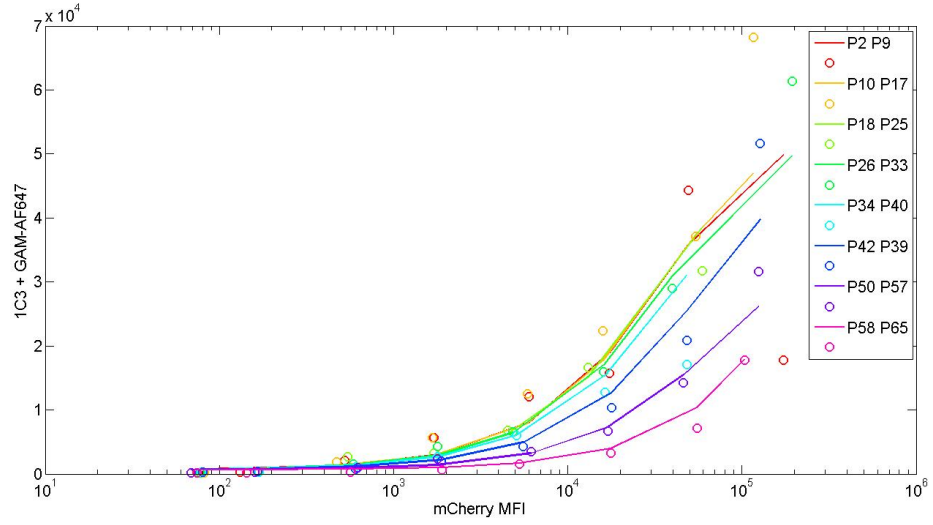# 2 150520-ASN-SSL-IFN-ifn1

2.1 Attempt 1

Here the data for SSL + 1ul IFN-gamma at the cell surface and ASN + 1ul IFN-gamma at the cell surface are fitted separately but with the same scale factors for the SSL and ASN cytoplasmic levels, sf1 and sf2 respectively. At this point gM=105.5 as normal and is not included in the fitting.

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

| Best Fit Scale Factors	
sf1	0.2339
sf2	0.9751
$p1_{MeSSL}$	0.0118
$p2_{MeSSL}$	647.2785
$p1_{MeASN}$	0.0003
$p2_{MeASN}$	148.1926
err	$4.8314e \times 10^{+04}$

(a)

(b)
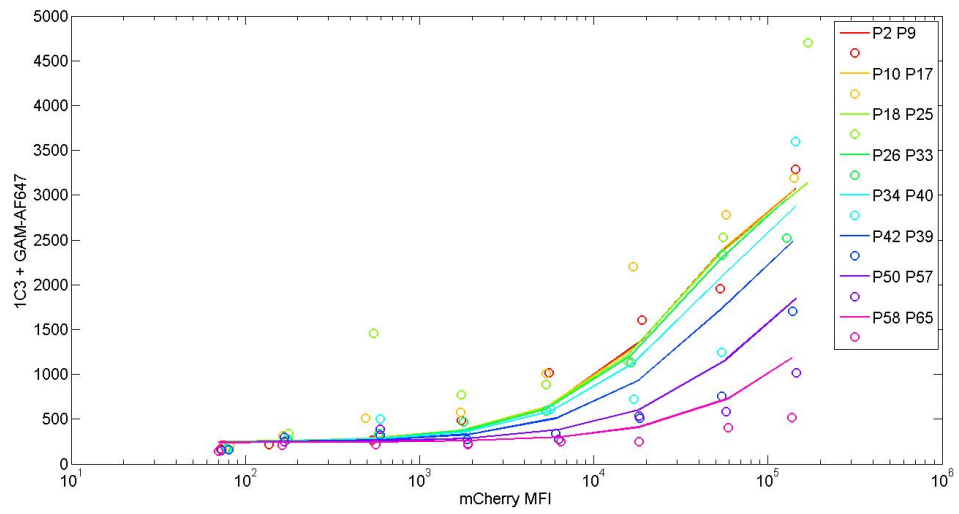
Figure 2

3
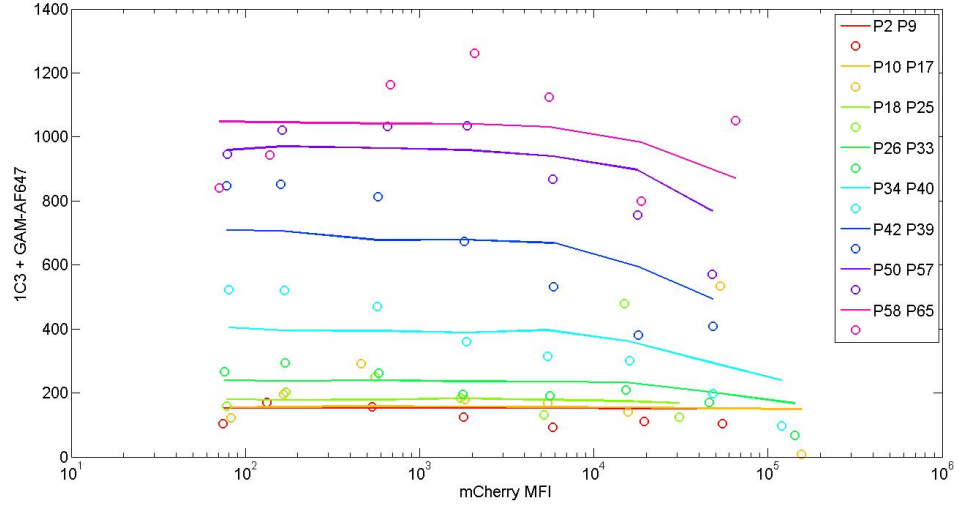
3   150520-ASN-SSL-IFN-both

3.1   Attempt 1

Here the data for SSL +/- 1ul IFN-gamma at the cell surface and ASN +/- 1ul IFN-gamma at the cell surface are fitted separately but with the same scale factors for the SSL and ASN cytoplasmic levels, sf1 and sf2 respectively. Additionally, for no IFN the parameter gM is fit for, whilst simultaneously fitting for upreg*gM for the with IFN data sets. A different polyfit is fit to each dataset. sf0=[1,1,1,1].

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

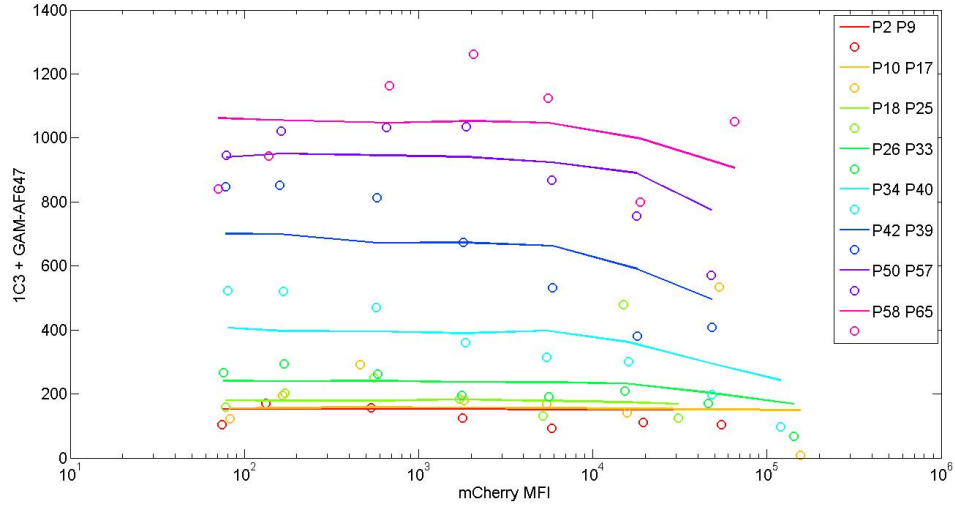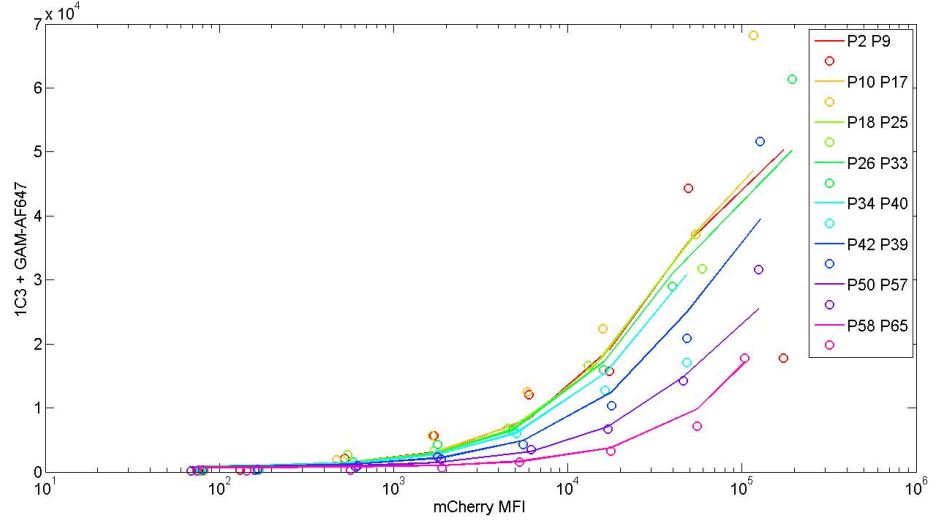| Best Fit Scale Factors	
sf1	0.2582
sf2	1.1255
gM1	11.3092
upreg	1.2563
$p1_{MeSSL_{n}one}$	0.0103
$p2_{MeSSL_{n}one}$	239.4523
$p1_{MeASN_{n}one}$	0.0002
$p2_{MeASN_{n}one}$	155.6190
$p1_{MeSSL_{i}fn}$	0.1279
$p2_{MeSSL_{i}fn}$	700.7013
$p1_{MeASN_{i}fn}$	0.0035
$p2_{MeASN_{i}fn}$	147.9339
err	$5.1998e \times 10^{+04}$
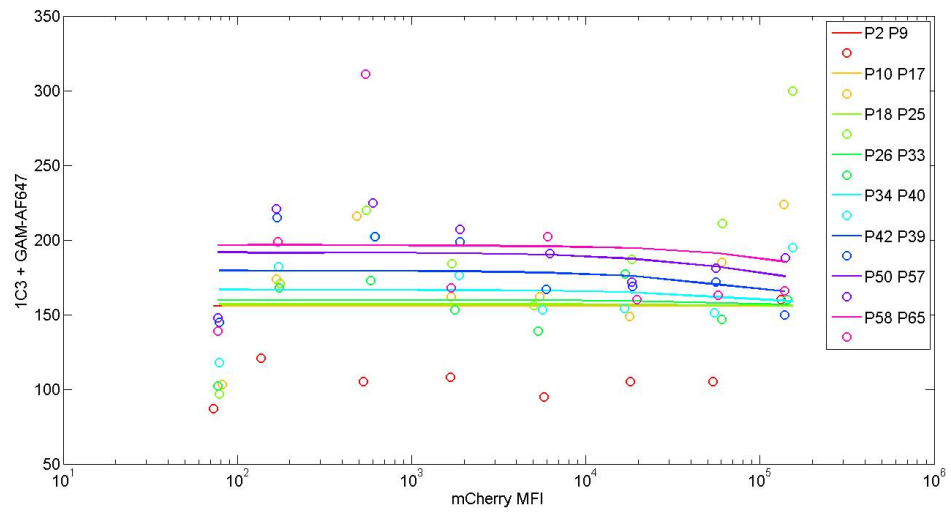
(a)

(b)
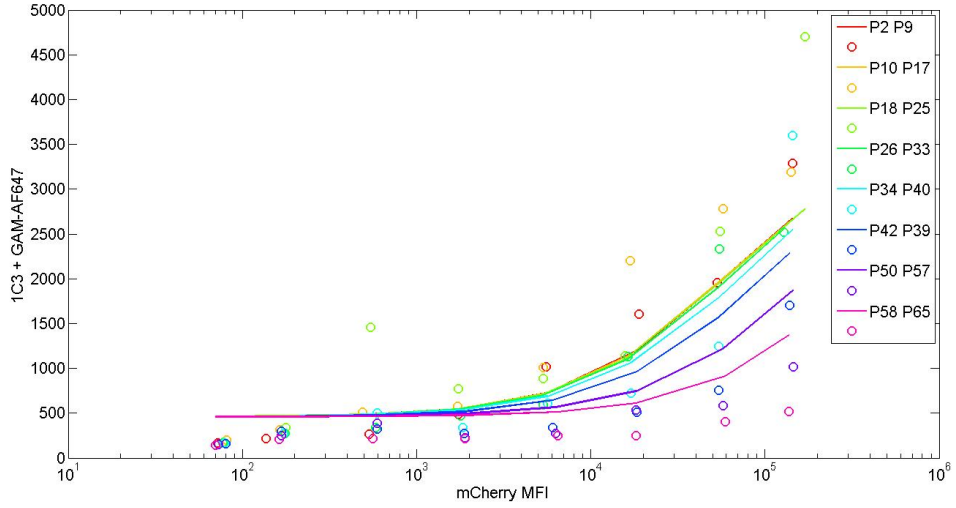
Figure 3

(a)

(b)

Figure 4

3.2 Attempt 2

Here the data for SSL +/- 1ul IFN-gamma at the cell surface and ASN +/- 1ul IFN-gamma at the cell surface are fitted separately but with the same scale factors for the SSL and ASN cytoplasmic levels, sf1 and sf2 respectively. Additionally, for no IFN the parameter gM is fit for, whilst simultaneously fitting for upreg*gM for the with IFN data sets. The same polyfit is used for the SSL surface data and the ASL surface data. sf1=[1,1,1,1].

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

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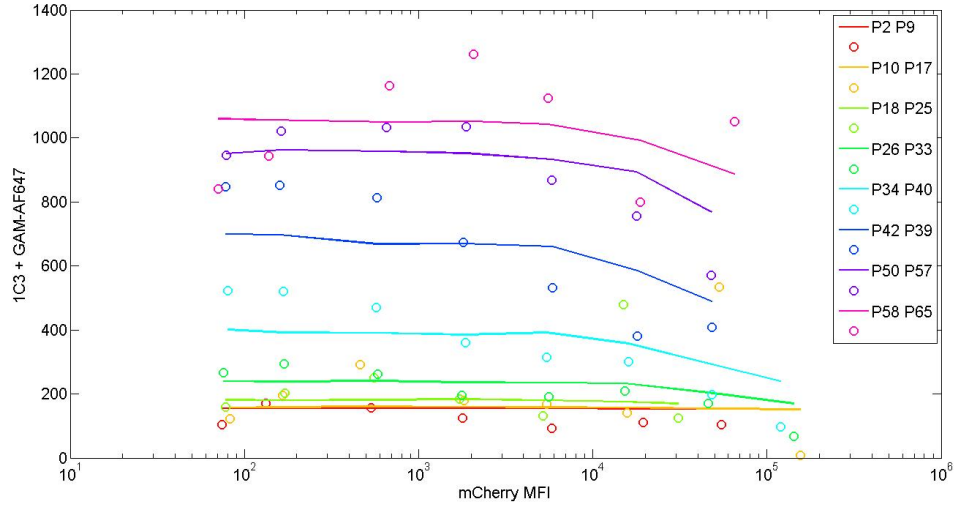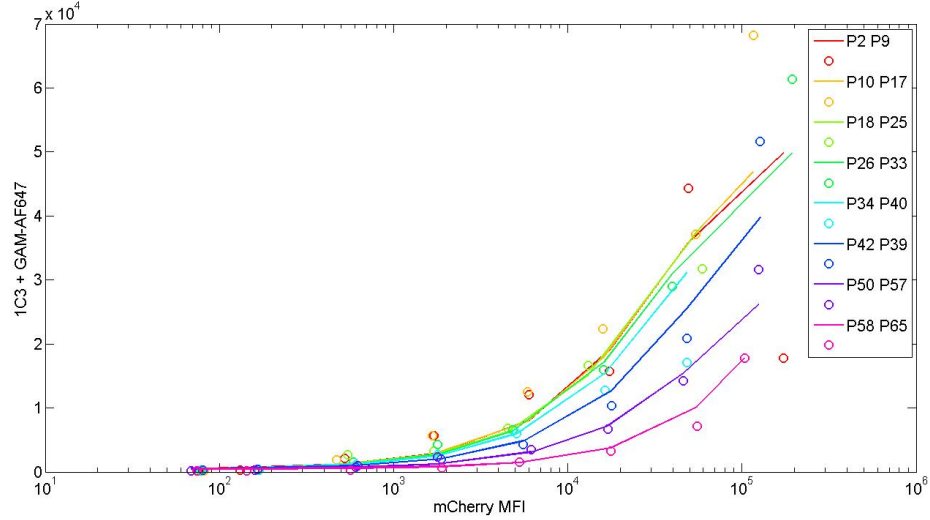| Best Fit Scale Factors	
sf1	0.2507
sf2	1.0090
gM1	2.7432
upreg	8.6576
$p1_{MeSSL_both}$	0.0656
$p2_{MeSSL_both}$	457.0106
$p1_{MeASN_both}$	0.0019
$p2_{MeASN_both}$	150.6764
err	$4.8492e \times 10^{+04}$
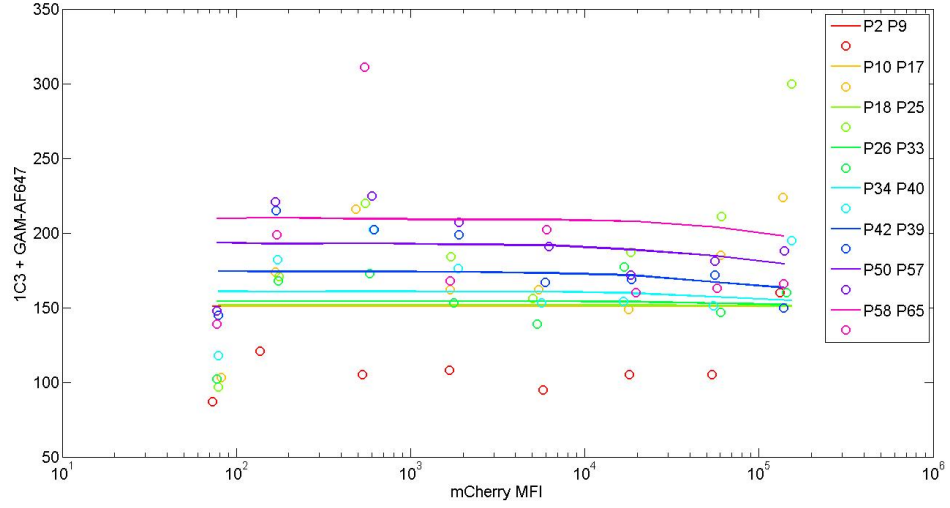
(a)

(b)

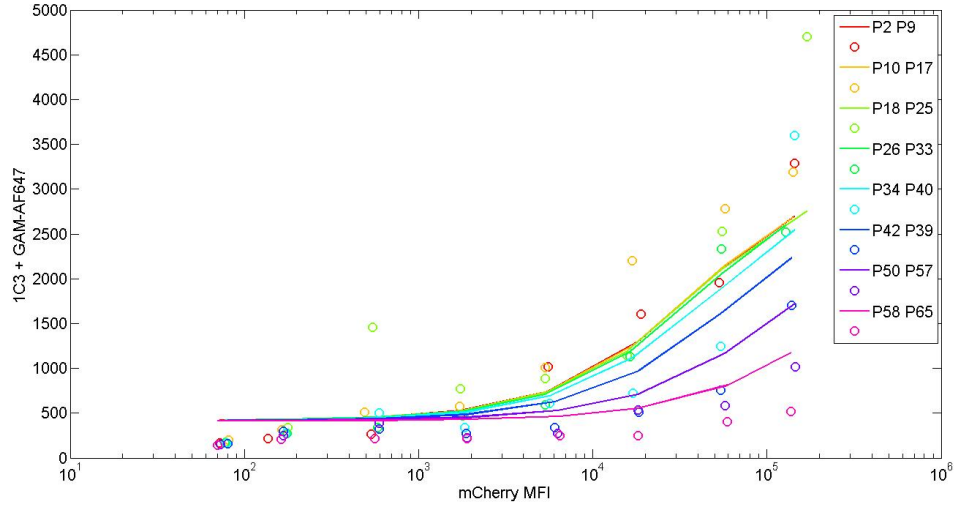Figure 5

(a)

(b)

Figure 6

3.3 Attempt 3

Here the data for SSL +/- 1ul IFN-gamma at the cell surface and ASN +/- 1ul IFN-gamma at the cell surface are fitted separately but with the same scale factors for the SSL and ASN cytoplasmic levels, sf1 and sf2 respectively. Additionally, for no IFN the parameter gM is fit for, whilst simultaneously fitting for upreg*gM for the with IFN data sets. The same polyfit is used for the SSL surface data and the ASL surface data. sf1=[1,1,1,1].

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

8

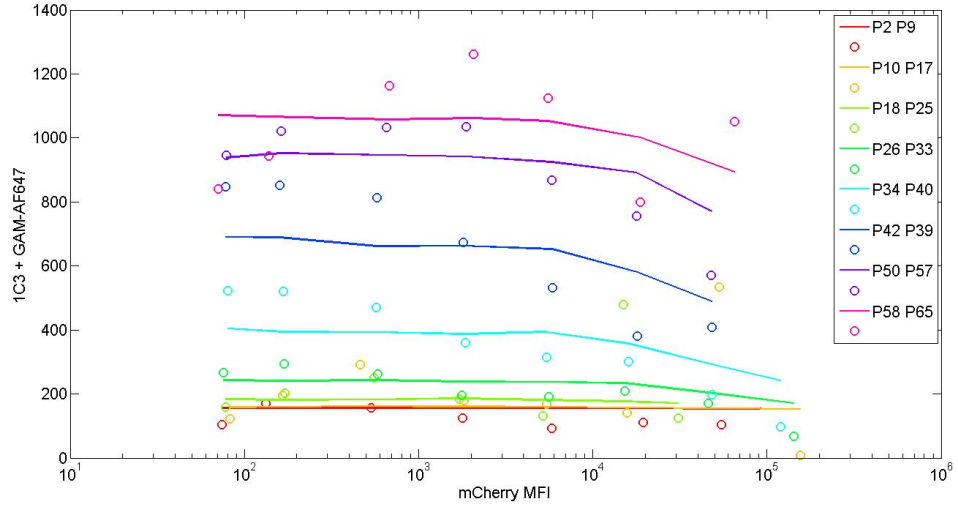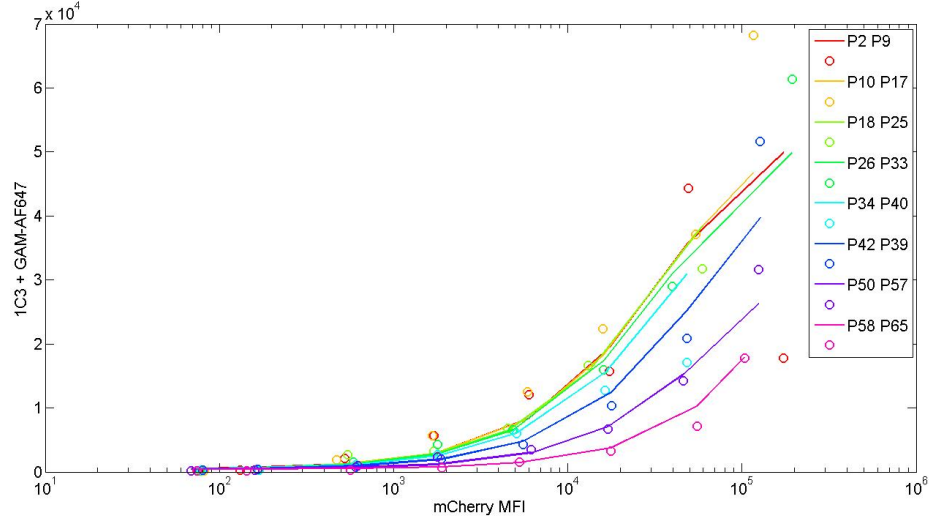| Best Fit Scale Factors	
sf1	1.3095
sf2	5.4970
gM1	53.9457
upreg	17.2416
$p1_{MeSSL_{both}}$	0.0041
$p2_{MeSSL_{both}}$	414.6326
$p1_{MeASN_{both}}$	0.0001
$p2_{MeASN_{both}}$	151.6457
err	$4.8377 \times 10^{+04}$
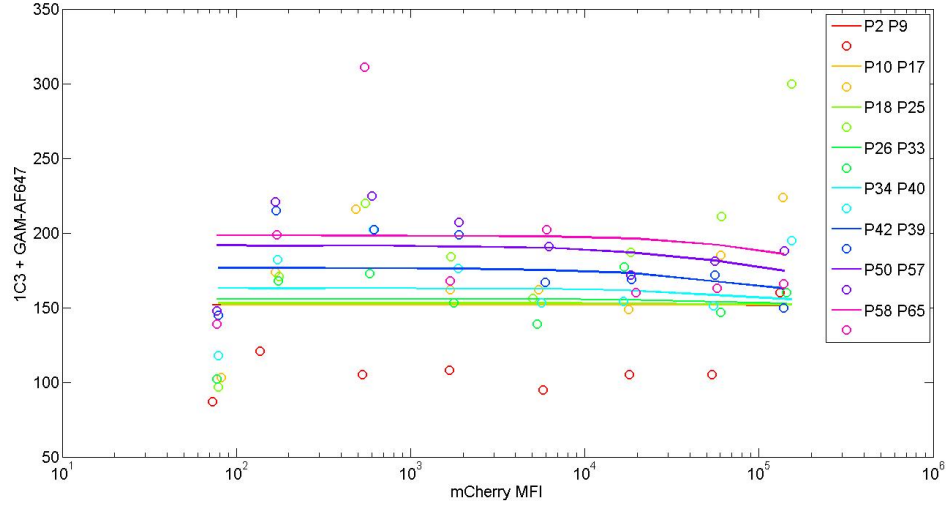
(a)

(b)

Figure 7

(a)

(b)

Figure 8

3.4 Attempt 4

Here the data for SSL +/- 1ul IFN-gamma at the cell surface and ASN +/- 1ul IFN-gamma at the cell surface are fitted separately but with the same scale factors for the SSL and ASN cytoplasmic levels, sf1 and sf2 for - IFN and upreg*sf1 and upreg*sf2 for + IFN. Additionally, for no IFN the parameter gM is fit for, whilst simultaneously fitting for upreg*gM for the with IFN data sets. The same polyfit is used for the SSL surface data and the ASL surface data. sf1=[1,1,1,1].

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

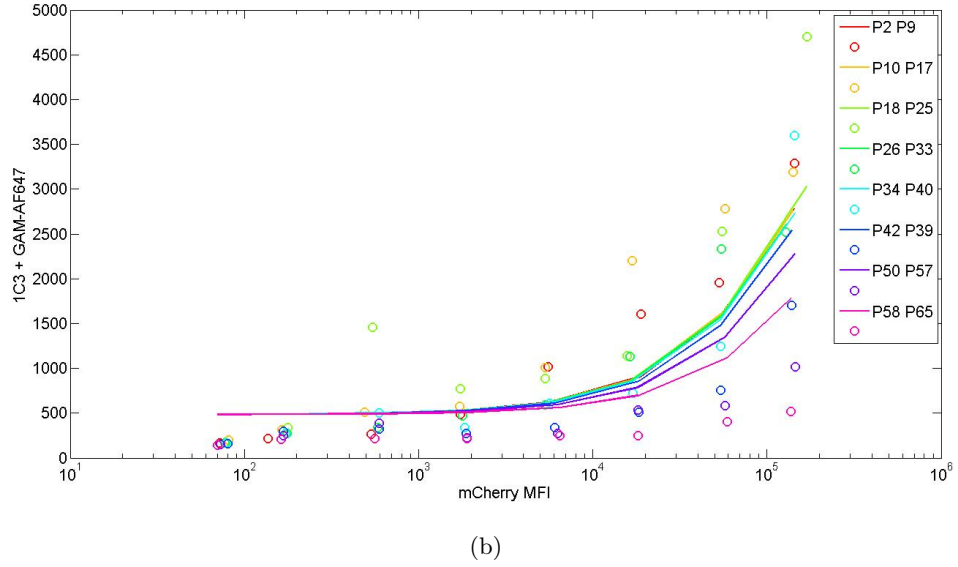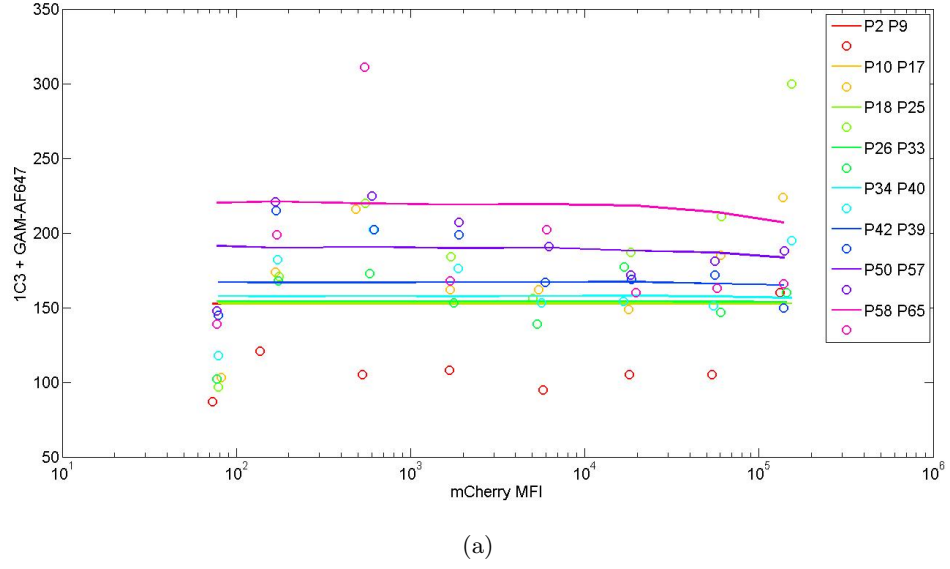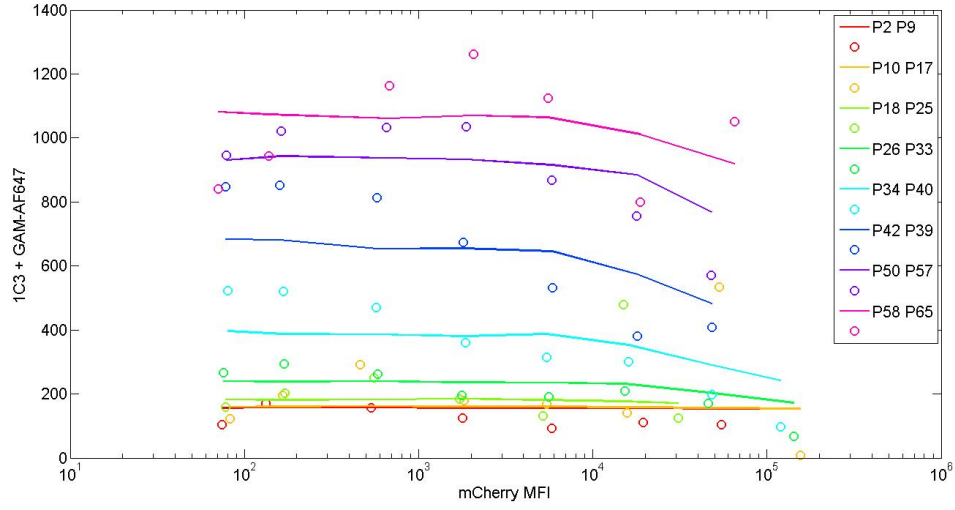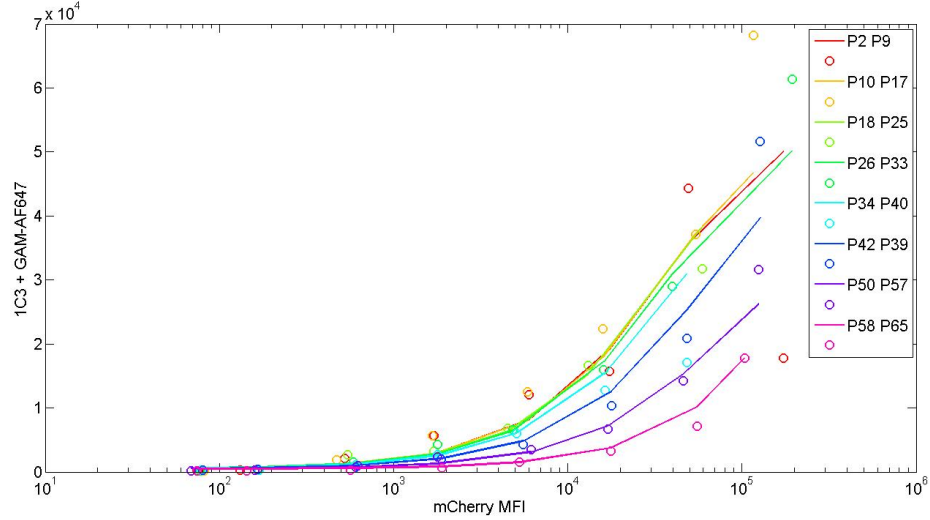| Best Fit Scale Factors	
sf1	0.0575
sf2	0.2297
gM1	2.1895
upreg	4.7387
$p1_{MeSSL_both}$	0.1951
$p2_{MeSSL_both}$	484.7132
$p1_{MeASN_both}$	0.0053
$p2_{MeASN_both}$	152.5158
err	$4.8572 \times 10^{+04}$

(a)

(b)

Figure 9

(a)

(b)

Figure 10

3.5 Attempt 5

Here the data for SSL +/- 1ul IFN-gamma at the cell surface and only ASN + 1ul IFN-gamma at the cell surface are fitted separately but with the same scale factors for the SSL and ASN cytoplasmic levels, sf1 and sf2 for - IFN and upreg*sf1 and upreg*sf2 for + IFN. Additionally, for no IFN the parameter gM is fit for, whilst simultaneously fitting for upreg*gM for the with IFN data sets. The same polyfit is used for the SSL surface data and the ASL surface data. sf1=[1,1,1,1].

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

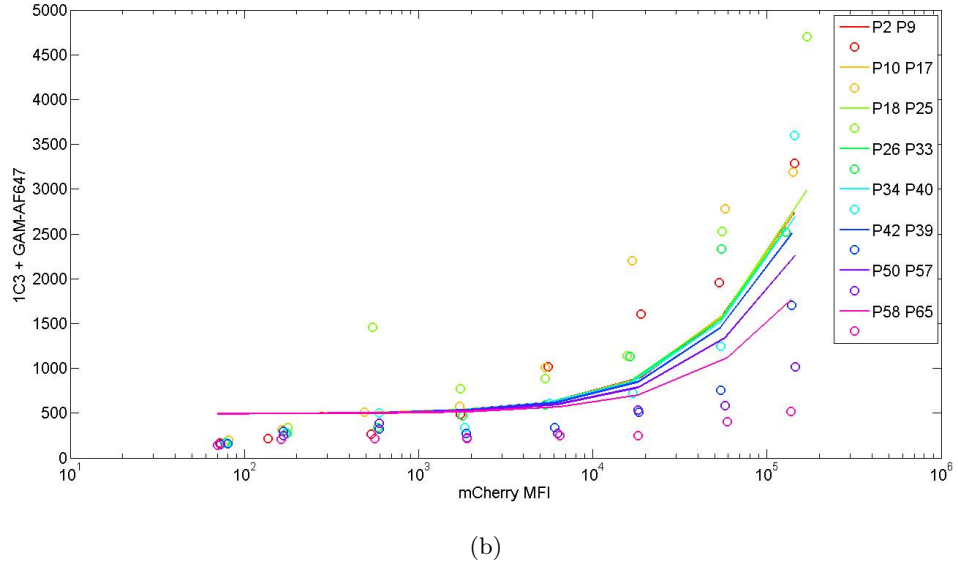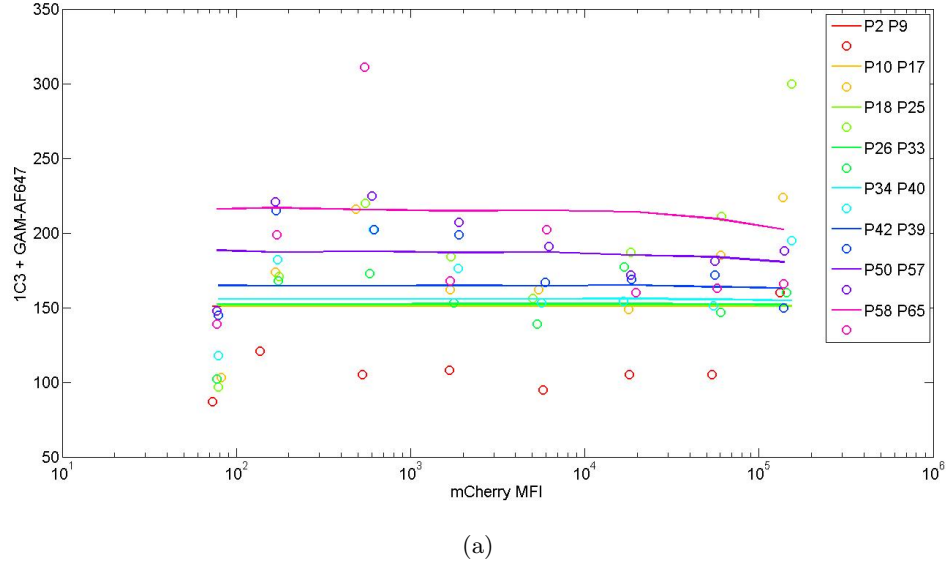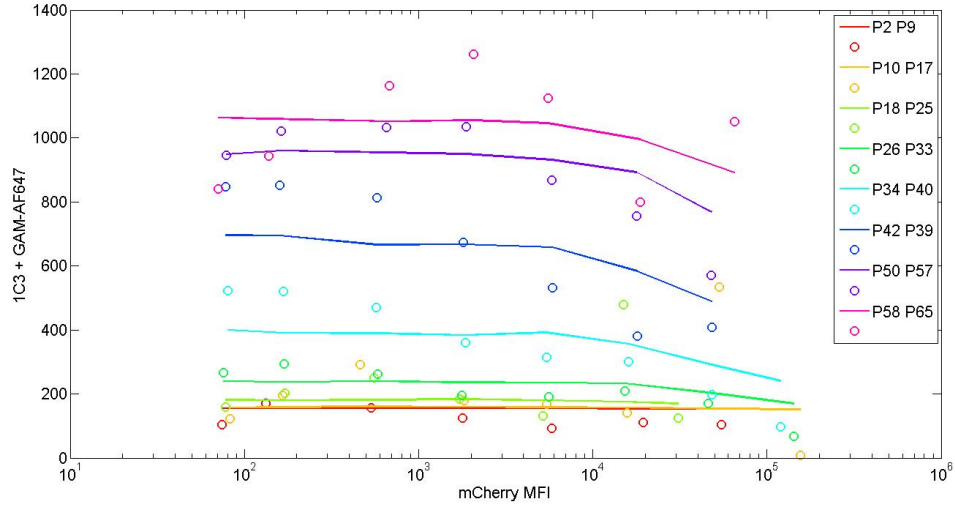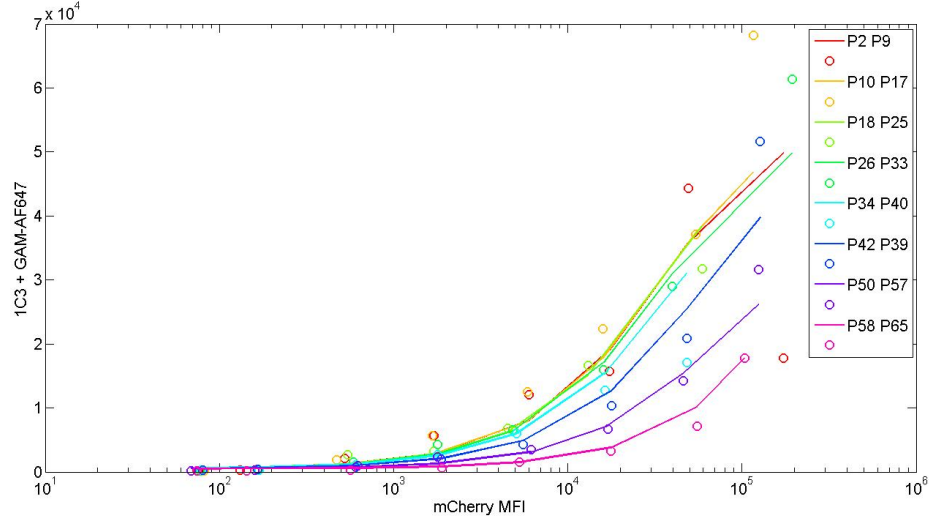| Best Fit Scale Factors	
sf1	0.0494
sf2	0.1985
gM1	3.8691
upreg	5.1344
$p1_{MeSSL_{both}}$	0.0822
$p2_{MeSSL_{both}}$	493.4132
$p1_{MeASN_{both}}$	0.0023
$p2_{MeASN_{both}}$	150.7901
err	$4.8509 \times 10^{+04}$

(a)

(b)

Figure 11

(a)

(b)

Figure 12

3.6   Attempt 6

Here the data for SSL +/- 1ul IFN-gamma at the cell surface and only ASN + 1ul IFN-gamma at the cell surface are fitted separately but with the same scale factors for the SSL and ASN cytoplasmic levels. Additionally, for no IFN the parameter gM is fit for, whilst simultaneously fitting for upreg*gM for the with IFN data sets. The same polyfit is used for the SSL surface data and the ASL surface data. sf1=[1,1,1,1].

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

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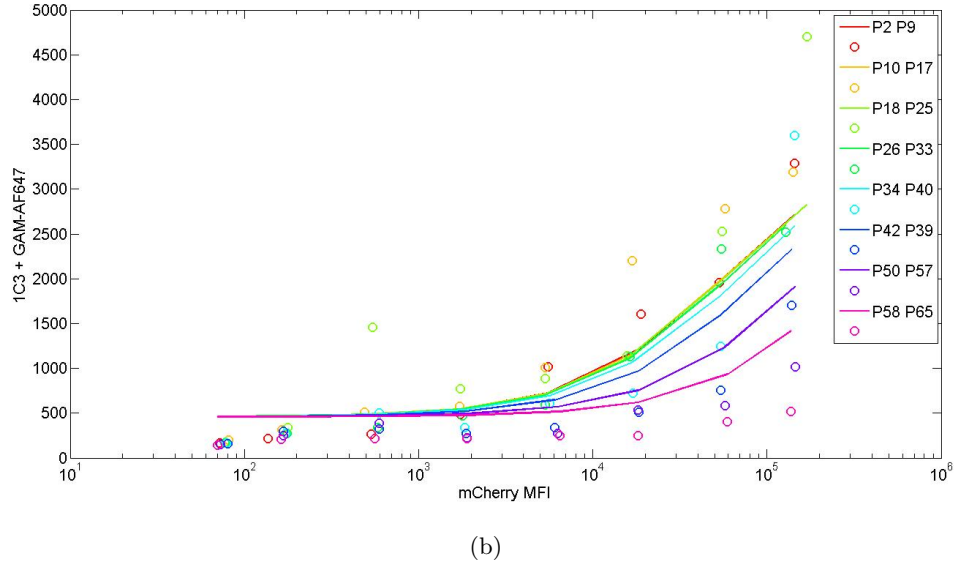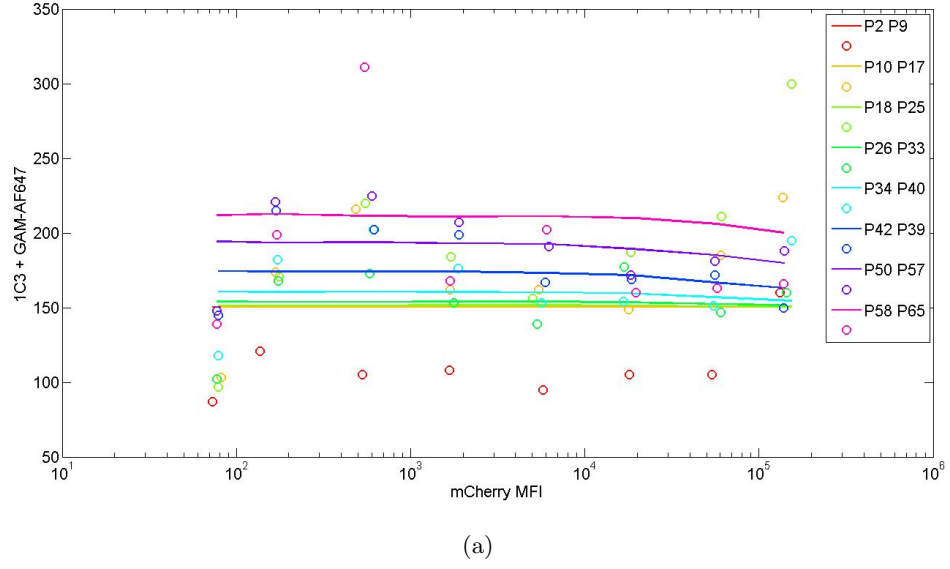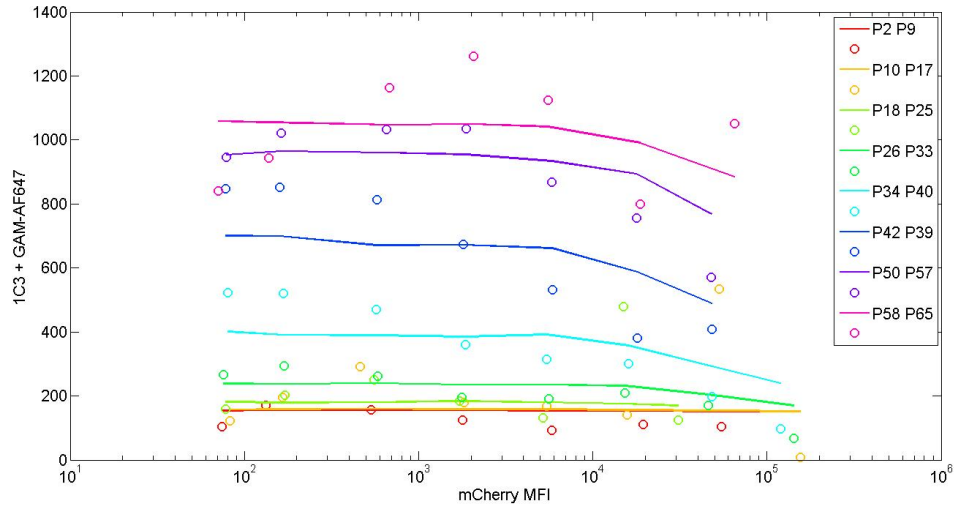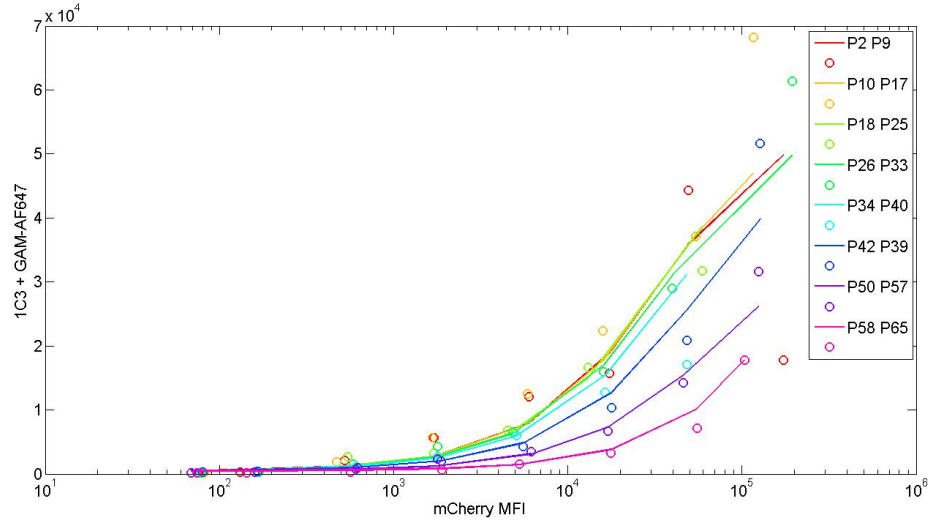| Best Fit Scale Factors	
sf1	0.2065
sf2	0.8302
gM1	2.0889
upreg	7.8689
$p1_{MeSSL_both}$	0.0949
$p2_{MeSSL_both}$	457.0403
$p1_{MeASN_both}$	0.0028
$p2_{MeASN_both}$	150.2214
err	$4.8476 \times 10^{+04}$

(a)

(b)

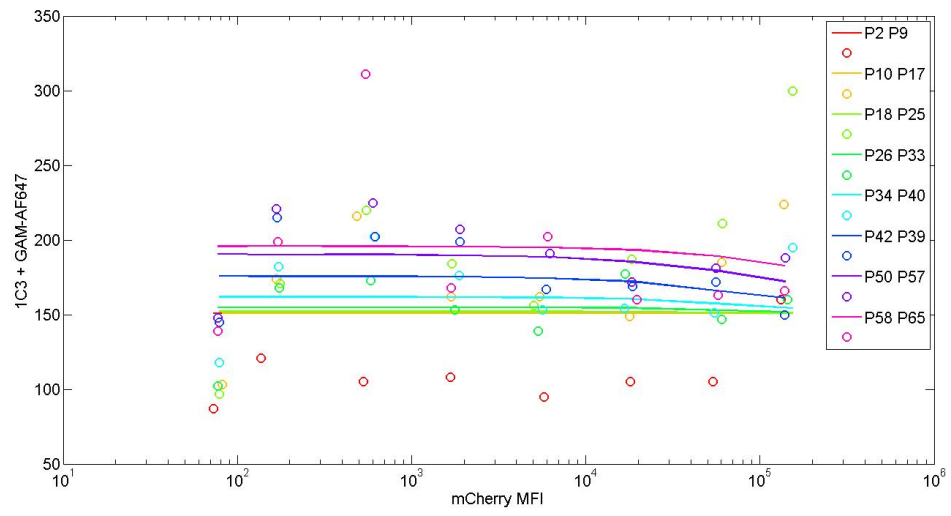Figure 13

(a)

(b)

Figure 14

4 Notes

- Removing ASN Surf - IFN data does not improve overall fit (although err is reduced because you are considering less datasets).

- When fitting for all data sets, including upregulation on gM only and not sf1 and sf2 seems to provide a better fit, especially for the - IFN data.

- It does not seem possible to get a particularly good fit to the ASN Surf - IFN data.

- The fits for the +IFN data appear to be much better than the -IFN data, this will be because the cell surface levels for the +IFN are much larger than the -IFN levels, and so greater minimisation of the total error will be achieved by getting at better fit to the +IFN data set at the expense of the - IFN data set. Perhaps we should introduce some kind of weighting or normalisation to the err calculation to reduce the bias in favour of the +IFN dataset?
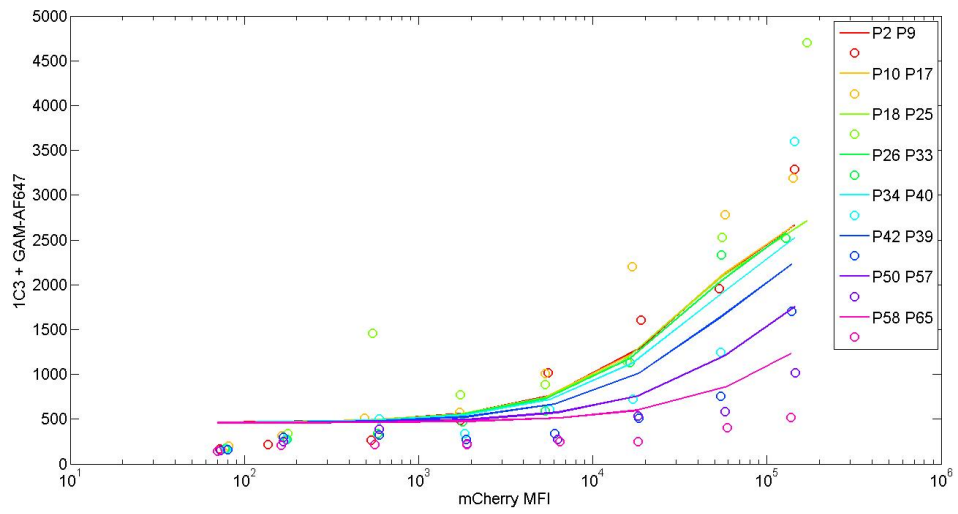
16

4.1 Attempt 7

Here the data for SSL +/- 1ul IFN-gamma at the cell surface and only ASN +/- 1ul IFN-gamma at the cell surface are fitted separately but with the same scale factors for the SSL and ASN cytoplasmic levels. Additionally, for no IFN the parameter gM is fit for, whilst simultaneously fitting for upreg*gM for the with IFN data sets. The same polyfit is used for the SSL surface data and the ASL surface data. sf1=[1,1,1,1].

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

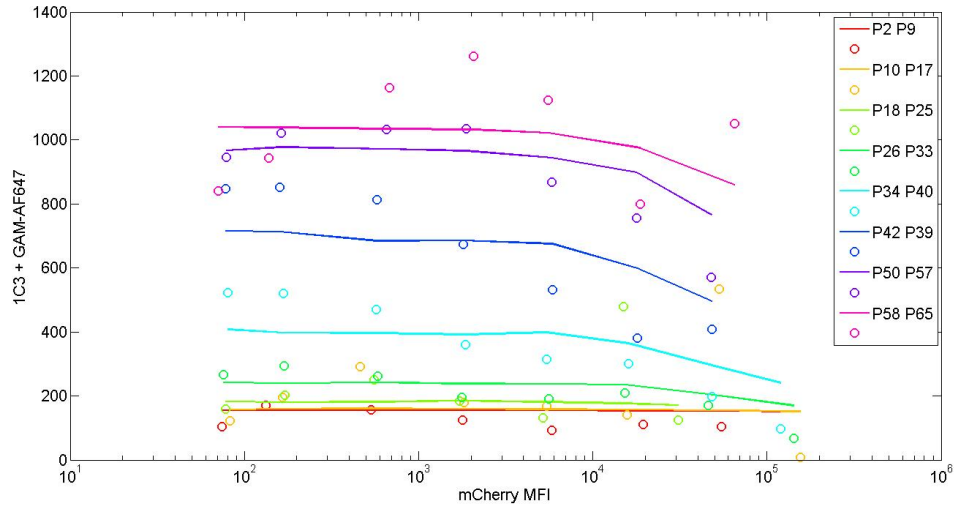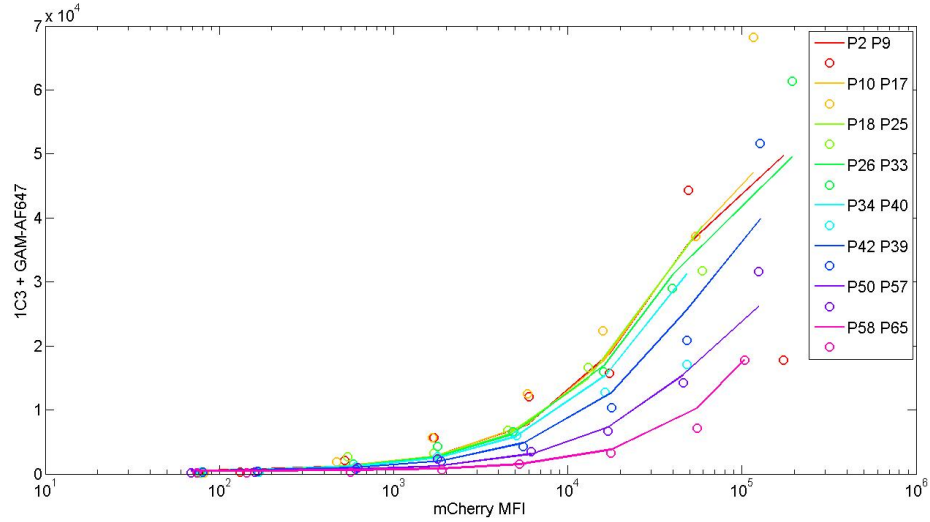| Best Fit Scale Factors	
sf1	0.1930
sf2	0.7928
gM1	9.8157
upreg	12.5608
$p1_{MeSSL_both}$	0.0089
$p2_{MeSSL_both}$	457.9798
$p1_{MeASN_both}$	0.0003
$p2_{MeASN_both}$	150.7687
err	$4.8494 \times 10^{+04}$

(a)

(b)

Figure 15

(a)

(b)

Figure 16

4.2 Attempt 8

Here the data for SSL +/- 1ul IFN-gamma at the cell surface and only ASN +/- 1ul IFN-gamma at the cell surface are fitted separately but with the same scale factors for the SSL and ASN cytoplasmic levels, but with upreg factor applied to sf1 and sf2 for + IFN. Additionally, for no IFN the parameter gM is fit for, whilst simultaneously fitting for upreg*gM for the with IFN data sets. The same polyfit is used for the SSL surface data and the ASL surface data. sf1=[1,1,1,1].

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

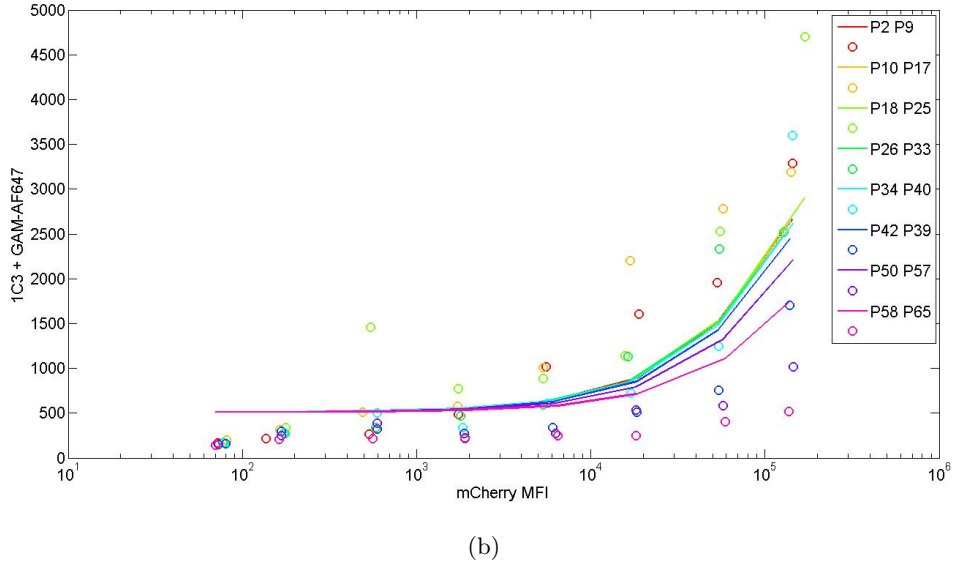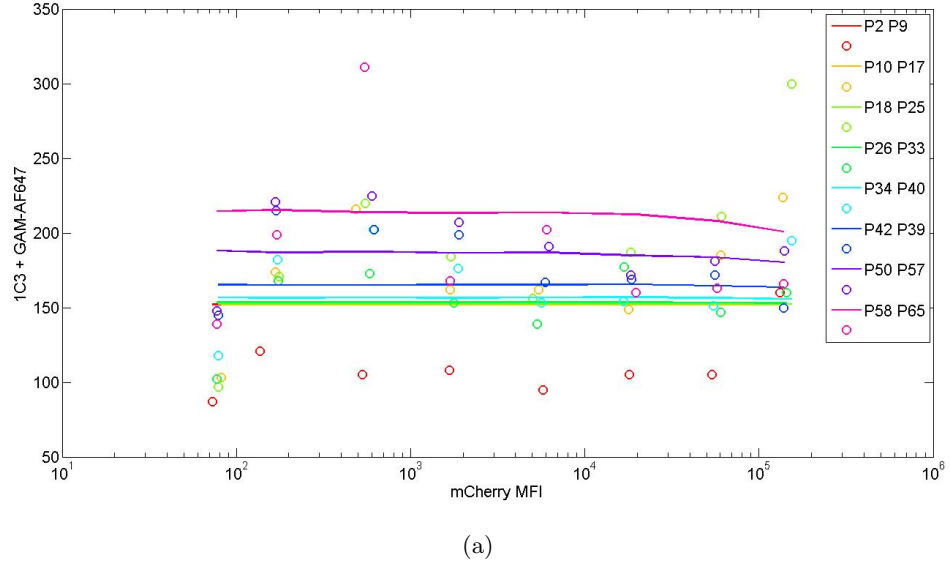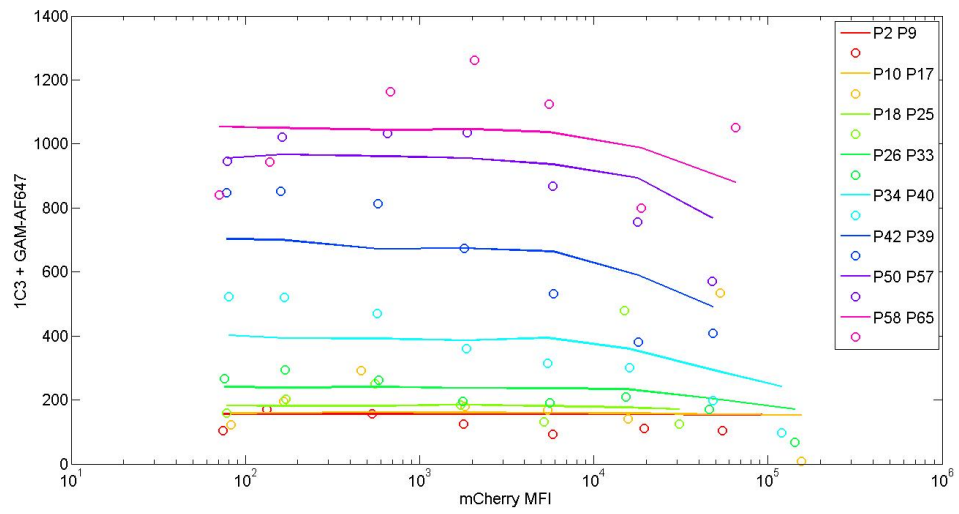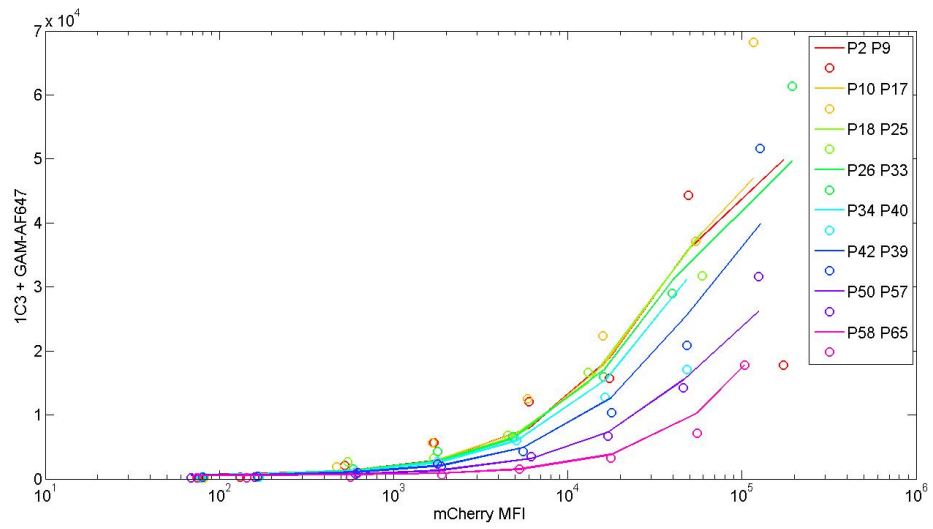| Best Fit Scale Factors	
sf1	0.0392
sf2	0.1583
gM1	3.7359
upreg	5.1918
$p1_{MeSSL_{both}}$	0.0764
$p2_{MeSSL_{both}}$	510.5382
$p1_{MeASN_{both}}$	0.0023
$p2_{MeASN_{both}}$	151.9069
err	$4.8494 \times 10^{+04}$

(a)

(b)

Figure 17

(a)

(b)

Figure 18