Supplement C: Fitted Parameters

In this Supplement, we analyze how to generate the shells one by one. And list their parameters. In order to do that, we first discuss the notation for the parameters. Take the parameters of *Furvus* as an example. Table S1 shows the vector notation for the parameters used in Matlab™. In the following, we first give the parameters for shells with basic patterns, then shells with spatial pre-pattern, and finally shells with spatio-temporal pre-patterns. We use hidden networks to generate spatio-temporal pre-patterns, so we also list the parameters of the hidden network(s).

S_1_e=[1 8 0.42]	$[\gamma^{(1)},\ \nu^{(1)},\ \theta^{(1)}]$	Sensory cell's sigmoid function
S_2_e=[1 6.7 0.033]	$[\gamma_e^{(2)},\ \nu_e^{(2)},\ \theta_e^{(2)}]$	Excitatory neuron's sigmoid function
S_2_i=[1 8.3 0.074]	$[\gamma_h^{(2)},\ \nu_h^{(2)},\ \theta_h^{(2)}]$	Inhibitory neuron's sigmoid function
S_3_e=[1 31 0.37]	$[\gamma^{(3)},\ \nu^{(3)},\ \theta^{(3)}]$	Secretory cell's sigmoid function
SF_2_e=[5 0.006]	$[\alpha_e,\ \sigma_e]$	Excitatory neuron's spatial kernel
SF_2_i=[1 0.018]	$[\alpha_h,\ \sigma_h]$	Inhibitory neuron's spatial kernel
TF_2_e=[5 0.02 4 0.01]	$[\beta_{e1}, c_{e1}, \beta_{e2}, c_{e2}]$	Excitatory neuron's temporal kernel
TF_2_i=[1.2 0.15 0.2 0.14]	$[\beta_{h1}, c_{h1}, \beta_{h2}, c_{h2}]$	Inhibitory neuron's temporal kernel

Table S1 The notations of the parameters. We always set $\gamma^{(1)} = \gamma_e^{(2)} = \gamma_h^{(2)} = \gamma^{(3)} = \alpha_h = 1$, and $\beta_{e1} = \beta_{e2} + 1$, $\beta_{h1} = \beta_{h2} + 1$ in our simulations. So we have 17 free parameters.

1.1 Shells with Basic Patterns

Furvus has in-phase checkerboard pattern.

```
S_1_e  = [1       8.      0.42];
S_2_e  = [1       6.7     0.033];
S_2_i  = [1       8.3     0.074];
S_3_e  = [1       31      0.37];
SF_2_e = [5       0.006];
SF_2_i = [1       0.018];
TF_2_e = [5       0.02    4       0.01];
TF_2_i = [1.20    0.15    0.20    0.14];
```

Consors has Turing strips.

```
S_1_e  = [1       10      0.35];
S_2_e  = [1       5       0.2];
S_2_i  = [1       10      0.15];
S_3_e  = [1       6       0.1];
SF_2_e = [1.5     0.06];
SF_2_i = [1       0.13];
TF_2_e = [1       0       0       0];
TF_2_i = [1       0       0       0];
```

Marmoreus has triangles.

```
S_1_e  = [1       15      0.25];
S_2_e  = [1       10      0.17];
S_2_i  = [1       20      0.35];
S_3_e  = [1       40      0.1];
```

```
SF_2_e = [6        0.01];
SF_2_i = [1        0.18];
TF_2_e = [3.79     0.45     2.79     0.56];
TF_2_i = [2.47     0.03     1.47     0.25];
```

Bandanus has more and smaller triangles than *marmoreus* does. So *bandanus* has narrower spatial kernels.

```
S_1_e  = [1        15       0.25];
S_2_e  = [1        10       0.17];
S_2_i  = [1        20       0.35];
S_3_e  = [1        40       0.1];
SF_2_e = [6        0.007];
SF_2_i = [1        0.12];
TF_2_e = [3.79     0.45     2.79     0.56];
TF_2_i = [2.47     0.03     1.47     0.25];
```

Omaria has travelling waves.

```
S_1_e  = [1        15       0.28];
S_2_e  = [1        14       0.17];
S_2_i  = [1        12.7     0.1];
S_3_e  = [1        25       0.1];
SF_2_e = [5        0.0065];
SF_2_i = [1        0.007];
TF_2_e = [3.665    0.21     2.665    0.33];
TF_2_i = [1.2      0.085    0.2      0.18];
```

Gloriamaris has more dense travelling waves, so its spatial kernel is narrower than that of *omaria.*

```
S_1_e  = [1        15       0.28];
S_2_e  = [1        14       0.17];
S_2_i  = [1        12.7     0.1];
S_3_e  = [1        19.5     0.1];
SF_2_e = [4.5      0.005];
SF_2_i = [1        0.007];
TF_2_e = [3.665    0.21     2.665    0.33];
TF_2_i = [1.2      0.085    0.2      0.18];
```

Pulicarius has dots.

```
S_1_e  = [1        15       0.3];
S_2_e  = [1        5        0.1];
S_2_i  = [1        5        0.06];
S_3_e  = [1        8        0.15];
SF_2_e = [3.5      0.02];
SF_2_i = [1        0.055];
TF_2_e = [2.28     0        1.28     0.32];
TF_2_i = [1.78     0        0.78     0.32];
```

Arenatus has smaller and more dots than *pulicarius* does. So *arenatus* has narrower spatial kernels.

```
S_1_e  = [1        15       0.3];
S_2_e  = [1        5        0.1];
S_2_i  = [1        5        0.06];
S_3_e  = [1        8        0.15];
SF_2_e = [3.5      0.0044];
SF_2_i = [1        0.012];
TF_2_e = [2.28     0        1.28     0.32];
TF_2_i = [1.78     0        0.78     0.32];
```

Crocatus has fewer dots than *pulicarius* does. So *crocatus* has wider spatial kernels.

```
S_1_e  = [1        15       0.3];
S_2_e  = [1        5        0.1];
S_2_i  = [1        5        0.06];
S_3_e  = [1        7.9      0.14];
SF_2_e = [3.5      0.02];
SF_2_i = [1        0.1];
TF_2_e = [2.28     0        1.28     0.32];
TF_2_i = [1.78     0        0.78     0.32];
```

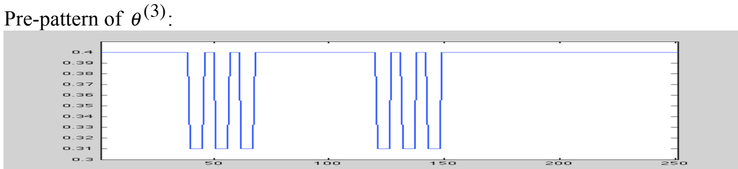
1.2 Shells with Spatial Pre-pattern

The parameter $\theta^{(3)}$, the middle point of the secretory cells' sigmoid functions, shown in this section has a spatial pre-pattern. We show its basic value as did in previous section. Moreover, we show the spatial pre-pattern of $\theta^{(3)}$.

Tessulatus's main pattern is out-phase checkerboard. But at some stripe regions, the checker has different color. At these strip regions, parameter $\theta^{(3)}$ is different.

```
S_1_e  = [1       8       0.42];
S_2_e  = [1       6.7     0.033];
S_2_i  = [1       8.3     0.074];
S_3_e  = [1       30      0.4];
SF_2_e = [5       0.015];
SF_2_i = [1       0.029];
TF_2_e = [5       0.02    4       0.01];
TF_2_i = [1.20    0.15    0.20    0.14];
```

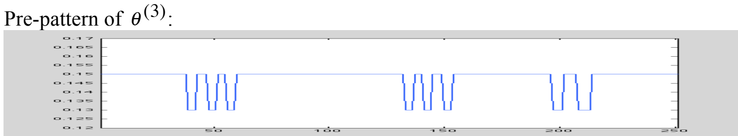
Pre-pattern of $\theta^{(3)}$:



Aurisiacus's main pattern is dots. But there are also stripes. At these strip regions, parameter $\theta^{(3)}$ is different.

```
S_1_e  = [1       15      0.3];
S_2_e  = [1       5       0.1];
S_2_i  = [1       5       0.06];
S_3_e  = [1       8       0.15];
SF_2_e = [3.1     0.015];
SF_2_i = [1       0.041];
TF_2_e = [2.28    0       1.28    0.3];
TF_2_i = [1.78    0       0.78    0.29];
```

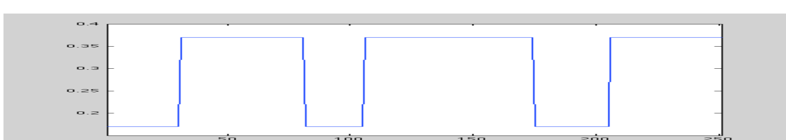
Pre-pattern of $\theta^{(3)}$:



Ammiralis's main pattern is triangles. And there are stripes. At these strip regions, parameter $\theta^{(3)}$ is different.

```
S_1_e  = [1       15      0.19];
S_2_e  = [1       17      0.3];
S_2_i  = [1       3       0.54];
S_3_e  = [1       20      0.37];
SF_2_e = [5       0.008];
SF_2_i = [1       0.041];
TF_2_e = [3.96    0       2.96    0.17];
TF_2_i = [6.82    0       5.82    0.04];
```

Pre-pattern of $\theta^{(3)}$:

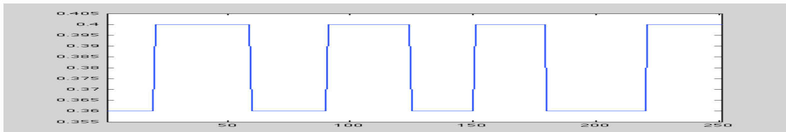


Orbignyi's main pattern is oscillating Turing-Hopf bifurcation. But at some stripe regions, the checkers have different color. At these strip regions, parameter $\theta^{(3)}$ is different.

```
S_1_e  = [1       8       0.42];
S_2_e  = [1       6.7     0.033];
S_2_i  = [1       8.3     0.074];
```

```
S_3_e  = [1        30       0.4];
SF_2_e = [5        0.008];
SF_2_i = [1        0.015];
TF_2_e = [5        0.02     4        0.01];
TF_2_i = [1.20     0.15     0.20     0.14];
```

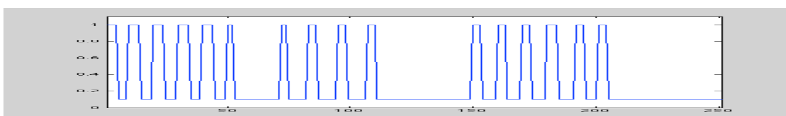
Pre-pattern of $\theta^{(3)}$:



Laterculatus's main pattern is oscillations. But at some stripe regions, the oscillations disappear. At these strip regions, parameter $\theta^{(3)}$ is different. We may also view this pattern as oscillating Turing-Hopf bifurcation, but the parameter region is relatively small, because the Turing bifurcation in this case is not regular.

```
S_1_e  = [1        6        0.3];
S_2_e  = [1        5        0.01];
S_2_i  = [1        5        0.06];
S_3_e  = [1        5        0.1];
SF_2_e = [2.5      0.009];
SF_2_i = [1        0.03];
TF_2_e = [3.28     0        2.28     0.3];
TF_2_i = [2.58     0        1.58     0.4];
```

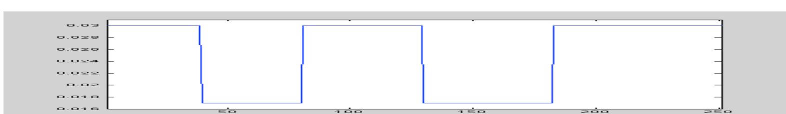
Pre-pattern of $\theta^{(3)}$:



Stercusmuscarum's main pattern is oscillating Turing-Hopf bifurcation. At some stripe regions, Turing bifurcation disappears, so only oscillations remain.

```
S_1_e  = [1        15       0.3];
S_2_e  = [1        5        0.1];
S_2_i  = [1        5        0.06];
S_3_e  = [1        22       0.03];
SF_2_e = [1.3      0.0067];
SF_2_i = [1        0.009];
TF_2_e = [2.28     0        1.28     0.3];
TF_2_i = [1.78     0        0.78     0.29];
```

Pre-pattern of $\theta^{(3)}$:



1.3 Shells with Spatio-temporal Pre-pattern

The parameter $v^{(3)}$, the slope of the middle point of the secretory cells' sigmoid functions, shown in this section has a spatio-temporal pre-pattern. We show its basic value as did in previous section. The pre-pattern of $v^{(3)}$ is generated by hidden network(s). So we also show the parameters of the hidden network(s), and the threshold functions used to couple visible networks and hidden networks.

Episcopatus's main pattern is travelling waves. And there are some patches.

Visible network (generate travelling waves and patches):

```
S_1_e  = [1        15       0.28];
S_2_e  = [1        14       0.17];
S_2_i  = [1        12.7     0.1];
S_3_e  = [1        19.5     0.1];
SF_2_e = [4        0.0065];
SF_2_i = [1        0.007];
```

```
TF_2_e = [3.665   0.21    2.665   0.33];
TF_2_i = [1.2     0.085   0.2     0.18];
```

Hidden network (generate patches):

```
S_1_e  = [1       15      0.3];
S_2_e  = [1       5       0.1];
S_2_i  = [1       5       0.06];
S_3_e  = [1       8       0.15];
SF_2_e = [2.5     0.01];
SF_2_i = [1       0.3];
TF_2_e = [2.28    0       1.28    0.33];
TF_2_i = [1.78    0       0.78    0.37];
```

Threshold function:

$$thres_1 = 0.2, a_1 = 0, \ b_1 = 5.7$$

Aulicus*'s* main pattern is travelling waves.

Visible network (generate travelling waves and patches):

```
S_1_e  = [1       15      0.28];
S_2_e  = [1       14      0.17];
S_2_i  = [1       12.7    0.1];
S_3_e  = [1       19.5    0.1];
SF_2_e = [4       0.006];
SF_2_i = [1       0.007];
TF_2_e = [3.665   0.21    2.665   0.33];
TF_2_i = [1.2     0.085   0.2     0.18];
```

Hidden network (generate patches):

```
S_1_e  = [1       15      0.3];
S_2_e  = [1       5       0.1];
S_2_i  = [1       5       0.06];
S_3_e  = [1       8       0.15];
SF_2_e = [2.5     0.01];
SF_2_i = [1       0.3];
TF_2_e = [2.28    0       1.28    0.33];
TF_2_i = [1.78    0       0.78    0.33];
```

Threshold function:

$$thres_1 = 0.2, a_1 = 0, \ b_1 = 7$$

Dalli*'s* main pattern is travelling waves. There are two spatio-temporal pre-patterns, i.e. oscillations and Turing stripes. They are generated by two independent hidden networks.

Visible network (generate travelling waves, Turing stripes and oscillations):

```
S_1_e  = [1       15      0.28];
S_2_e  = [1       14      0.17];
S_2_i  = [1       12.7    0.1];
S_3_e  = [1       19.5    0.1];
SF_2_e = [7       0.006];
SF_2_i = [1       0.007];
TF_2_e = [3.665   0.21    2.665   0.33];
TF_2_i = [1.2     0.085   0.2     0.18];
```

Hidden network1 (generate oscillations):

```
S_1_e  = [1       6       0.3];
S_2_e  = [1       5       0.01];
S_2_i  = [1       4       0.06];
S_3_e  = [1       3.5     0.1];
SF_2_e = [2.5     0.005];
SF_2_i = [1       0.2];
TF_2_e = [3.28    0       2.28    0.3];
TF_2_i = [2.58    0       1.58    0.4];
```

Hidden network2 (generate Turing stripes):

```
S_1_e  = [1       10      0.4];
S_2_e  = [1       5       0.2];
S_2_i  = [1       10      0.15];
S_3_e  = [1       6       0.1];
SF_2_e = [1.5     0.06];
SF_2_i = [1       0.241];
TF_2_e = [1       0       0       0];
TF_2_i = [1       0       0       0];
```

Threshold functions:

$$thres_1 = 0.3, a_1 = 0,\ b_1 = 5.5$$

$$thres_2 = 0.3, a_2 = 0,\ b_2 = 7$$

Textile is similar to *dalli.*

Visible network (generate travelling waves, Turing stripes and oscillations):

```
S_1_e  = [1       15      0.28];
S_2_e  = [1       14      0.17];
S_2_i  = [1       12.7    0.1];
S_3_e  = [1       19.5    0.1];
SF_2_e = [4.5     0.006];
SF_2_i = [1       0.007];
TF_2_e = [3.665   0.21    2.665   0.33];
TF_2_i = [1.2     0.085   0.2     0.18];
```

Hidden network1 (generate oscillations):

```
S_1_e  = [1       6       0.3];
S_2_e  = [1       5       0.01];
S_2_i  = [1       4       0.06];
S_3_e  = [1       3.5     0.1];
SF_2_e = [2.5     0.005];
SF_2_i = [1       0.2];
TF_2_e = [3.28    0       2.28    0.3];
TF_2_i = [2.58    0       1.58    0.4];
```

Hidden network2 (generate Turing stripes):

```
S_1_e  = [1       10      0.4];
S_2_e  = [1       5       0.2];
S_2_i  = [1       10      0.15];
S_3_e  = [1       6       0.1];
SF_2_e = [1.5     0.06];
SF_2_i = [1       0.241];
TF_2_e = [1       0       0       0];
TF_2_i = [1       0       0       0];
```

Threshold functions:

$$thres_1 = 0.3,\ a_1 = 0,\ b_1 = 5.5$$

$$thres_2 = 0.2, a_2 = 0,\ b_2 = 4.5$$

1.4 Inferred Ancestral Shells' Parameters

Number 20:

```
S_1_e  = [1       10.799  0.35];
S_2_e  = [1       5.936   0.085];
S_2_i  = [1       -7.855  0.107];
S_3_e  = [1       20.447  0.248];
SF_2_e = [4.244   0.012];
SF_2_i = [1       0.037];
TF_2_e = [3.836   0.065   2.836   0.17];
TF_2_i = [1.621   0.081   0.621   0.195];
```

Number 21:

```
S_1_e  = [1       12.017  0.319];
```

```
S_2_e  = [1       9.377   0.108];
S_2_i  = [1       5.901   0.121];
S_3_e  = [1       20.314  0.181];
SF_2_e = [3.915   0.014];
SF_2_i = [1       0.047];
TF_2_e = [3.33    0.084   2.33    0.24];
TF_2_i = [1.804   0.051   0.804   0.219];
```

Number 22:
```
S_1_e  = [1       12.236  0.318];
S_2_e  = [1       10.675  0.115];
S_2_i  = [1       8.032   0.137];
S_3_e  = [1       22.89   0.193];
SF_2_e = [4.304   0.013];
SF_2_i = [1       0.048];
TF_2_e = [3.583   0.113   2.583   0.247];
TF_2_i = [1.821   0.062   0.821   0.206];
```

Number 23:
```
S_1_e  = [1       12.856  0.307];
S_2_e  = [1       10.488  0.129];
S_2_i  = [1       9.367   0.157];
S_3_e  = [1       24.307  0.182];
SF_2_e = [4.551   0.011];
SF_2_i = [1       0.051];
TF_2_e = [3.643   0.147   2.643   0.277];
TF_2_i = [1.9     0.063   0.9     0.202];
```

Number 24:
```
S_1_e  = [1       13.354  0.3];
S_2_e  = [1       12.035  0.142];
S_2_i  = [1       7.041   0.151];
S_3_e  = [1       22.283  0.18];
SF_2_e = [4.644   0.009];
SF_2_i = [1       0.037];
TF_2_e = [3.702   0.141   2.702   0.269];
TF_2_i = [1.909   0.069   0.909   0.187];
```

Number 25:
```
S_1_e  = [1       14.026  0.283];
S_2_e  = [1       12.541  0.167];
S_2_i  = [1       2.056   0.175];
S_3_e  = [1       20.813  0.175];
SF_2_e = [4.848   0.008];
SF_2_i = [1       0.028];
TF_2_e = [3.717   0.148   2.717   0.277];
TF_2_i = [2.193   0.067   1.193   0.17];
```

Number 26:
```
S_1_e  = [1       14.425  0.268];
S_2_e  = [1       13.657  0.188];
S_2_i  = [1       4.523   0.212];
S_3_e  = [1       20.985  0.186];
SF_2_e = [5.102   0.008];
SF_2_i = [1       0.025];
TF_2_e = [3.741   0.141   2.741   0.274];
TF_2_i = [2.651   0.061   1.651   0.153];
```

Number 27:
```
S_1_e  = [1       14.62   0.272];
S_2_e  = [1       13.074  0.182];
S_2_i  = [1       9.359   0.174];
S_3_e  = [1       19.664  0.157];
SF_2_e = [5.322   0.007];
SF_2_i = [1       0.019];
TF_2_e = [3.715   0.164   2.715   0.293];
TF_2_i = [2.158   0.069   1.158   0.162];
```

Number 27 is assumed to have two hidden networks as its decedents do. We use phylogenetically independent contrasts method to infer the parameters of the two hidden networks.

Hidden network1:

```
S_1_e  = [1       6       0.3];
S_2_e  = [1       5       0.01];
S_2_i  = [1       4       0.06];
S_3_e  = [1       3.5     0.1];
SF_2_e = [2.5     0.005];
SF_2_i = [1       0.2];
TF_2_e = [3.28    0       2.28    0.3];
TF_2_i = [2.58    0       1.58    0.4];
```

Hidden network2:

```
S_1_e  = [1       10      0.4];
S_2_e  = [1       5       0.2];
S_2_i  = [1       10      0.15];
S_3_e  = [1       6       0.1];
SF_2_e = [1.5     0.06];
SF_2_i = [1       0.241];
TF_2_e = [1       0       0       0];
TF_2_i = [1       0       0       0];
```

Threshold functions:

$$thres_1 = 0.3, a_1 = 0, \ b_1 = 5.5$$

$$thres_2 = 0.25, a_2 = 0, \ b_2 = 5.75$$

Number 28:

```
S_1_e  = [1       13.185  0.31];
S_2_e  = [1       11.499  0.132];
S_2_i  = [1       12.518  0.125];
S_3_e  = [1       21.853  0.183];
SF_2_e = [4.546   0.009];
SF_2_i = [1       0.034];
TF_2_e = [3.738   0.13    2.738   0.255];
TF_2_i = [1.675   0.077   0.675   0.19];
```

Number 29:

```
S_1_e  = [1       14.012  0.299];
S_2_e  = [1       11.978  0.141];
S_2_i  = [1       14.718  0.108];
S_3_e  = [1       18.892  0.15];
SF_2_e = [4.359   0.01];
SF_2_i = [1       0.033];
TF_2_e = [3.532   0.14    2.532   0.288];
TF_2_i = [1.531   0.07    0.531   0.203];
```

Number 30:

```
S_1_e  = [1       14.08   0.298];
S_2_e  = [1       11.781  0.14];
S_2_i  = [1       15.007  0.106];
S_3_e  = [1       18.569  0.148];
SF_2_e = [4.352   0.01];
SF_2_i = [1       0.035];
TF_2_e = [3.493   0.138   2.493   0.29];
TF_2_i = [1.528   0.068   0.528   0.206];
```

Number 31:

```
S_1_e  = [1       14.417  0.291];
S_2_e  = [1       11.844  0.153];
S_2_i  = [1       10.032  0.105];
S_3_e  = [1       18.977  0.13];
SF_2_e = [4.212   0.008];
SF_2_i = [1       0.022];
```

```
TF_2_e = [3.587   0.169   2.587   0.305];
TF_2_i = [1.395   0.076   0.395   0.194];
```

Number 31 is assumed to have one hidden network.

Hidden network (generate patches):

```
S_1_e  = [1       15      0.3];
S_2_e  = [1       5       0.1];
S_2_i  = [1       5       0.06];
S_3_e  = [1       8       0.15];
SF_2_e = [2.5     0.01];
SF_2_i = [1       0.3];
TF_2_e = [2.28    0       1.28    0.33];
TF_2_i = [1.78    0       0.78    0.35];
```

Threshold function:

$$thres_1 = 0.2, a_1 = 0, b_1 = 6.35$$

Number 32:
```
S_1_e  = [1       14.823  0.255];
S_2_e  = [1       9.807   0.167];
S_2_i  = [1       19.971  0.334];
S_3_e  = [1       38.701  0.107];
SF_2_e = [5.88    0.009];
SF_2_i = [1       0.142];
TF_2_e = [3.778   0.425   2.778   0.537];
TF_2_i = [2.423   0.033   1.423   0.246];
```

Number 33:
```
S_1_e  = [1       11.98   0.316];
S_2_e  = [1       8.451   0.105];
S_2_i  = [1       5.623   0.108];
S_3_e  = [1       18.181  0.161];
SF_2_e = [3.519   0.016];
SF_2_i = [1       0.047];
TF_2_e = [3.034   0.06    2.034   0.243];
TF_2_i = [1.813   0.036   0.813   0.235];
```

Number 34:
```
S_1_e  = [1       11.711  0.312];
S_2_e  = [1       8.779   0.093];
S_2_i  = [1       7.91    0.096];
S_3_e  = [1       16.032  0.153];
SF_2_e = [3.401   0.014];
SF_2_i = [1       0.043];
TF_2_e = [2.96    0.045   1.96    0.26];
TF_2_i = [1.895   0.027   0.895   0.265];
```

Number 35:
```
S_1_e  = [1       14.359  0.302];
S_2_e  = [1       7.307   0.099];
S_2_i  = [1       5.719   0.067];
S_3_e  = [1       9.967   0.151];
SF_2_e = [3.481   0.013];
SF_2_i = [1       0.035];
TF_2_e = [2.413   0.009   1.413   0.308];
TF_2_i = [1.803   0.005   0.803   0.309];
```

Number 36:
```
S_1_e  = [1       12.609  0.318];
S_2_e  = [1       4.275   0.125];
S_2_i  = [1       1.819   0.101];
S_3_e  = [1       12.908  0.121];
SF_2_e = [2.572   0.024];
SF_2_i = [1       0.058];
TF_2_e = [2.287   0.024   1.287   0.207];
TF_2_i = [1.611   0.015   0.611   0.2];
```

Number 37:
```
S_1_e  = [1       13.691  0.31];
```

```
S_2_e  = [1       3.745   0.114];
S_2_i  = [1       8.045   0.082];
S_3_e  = [1       13.409  0.107];
SF_2_e = [2.404   0.018];
SF_2_i = [1       0.043];
TF_2_e = [2.284   0.013   1.284   0.249];
TF_2_i = [1.688   0.008   0.688   0.241];
```