

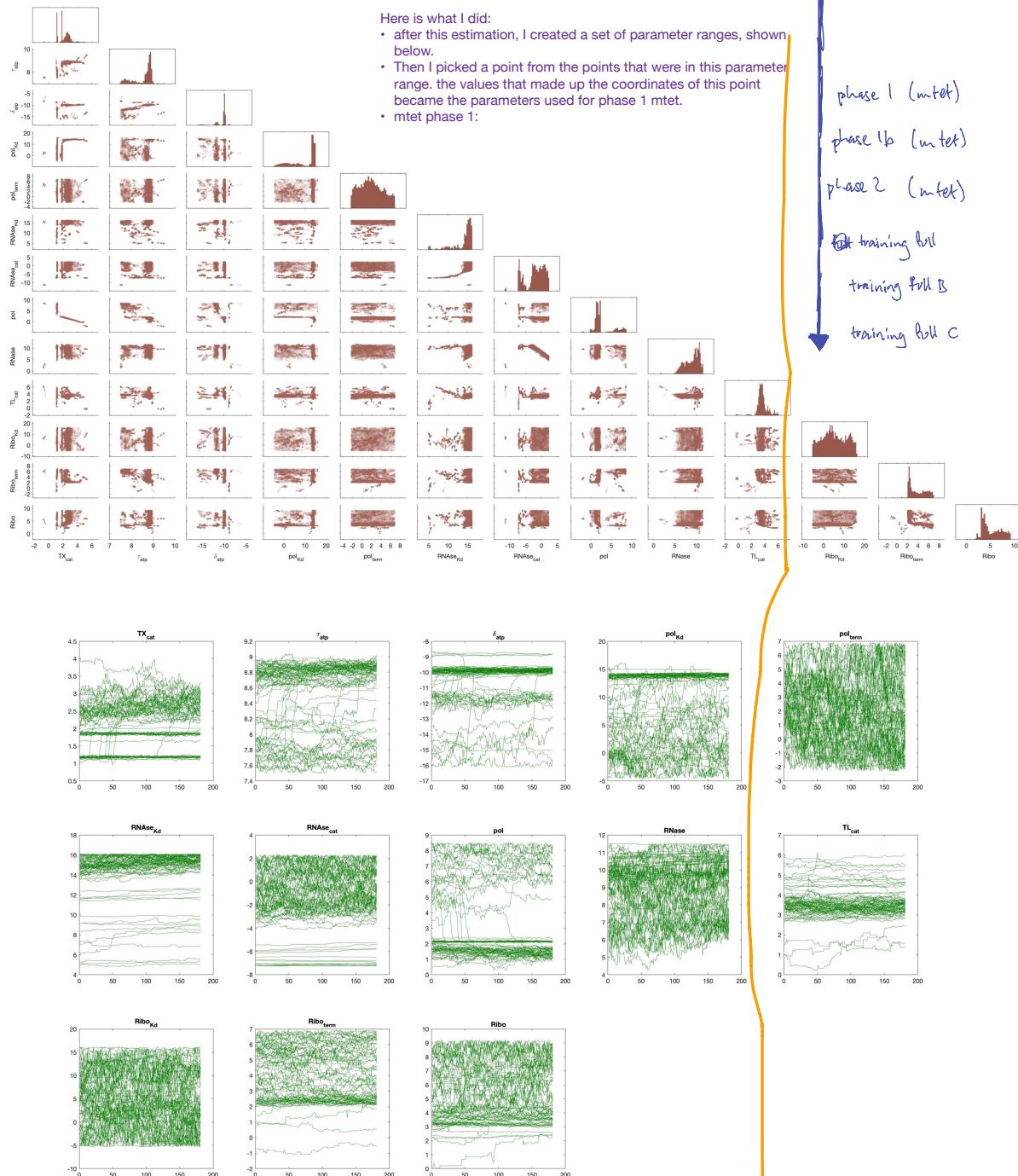
Overall, we can only effectively optimize up to 15 params. so we need to take a stepwise approach.

VNPRL

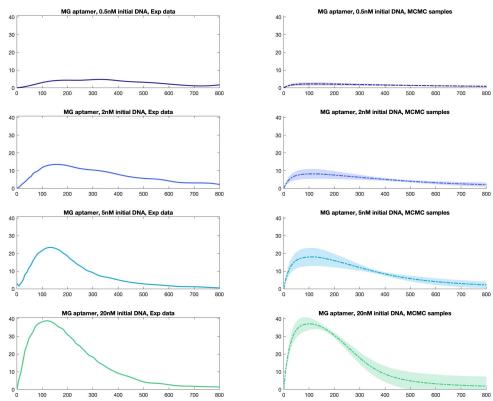
simdata\_20190223\_024333\_1\_2

/Users/vipulsinghal/Dropbox/Documents/toolbox/txtlsm\_vsfork2017/mcmc\_simbio/projects/proj\_vnprl/

MARL (F2)



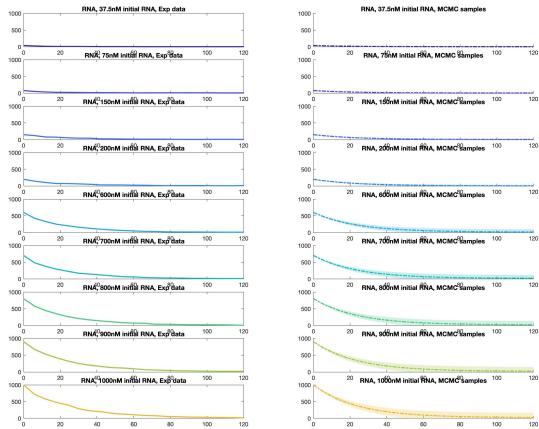
simdata\_20190223\_024333\_1\_2/cornerplot20190223\_024333\_1\_2BurnedIn.jpg



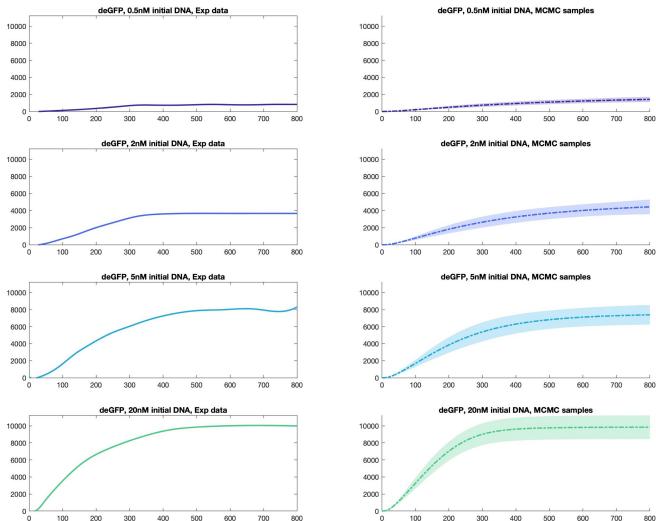
vnprl\_F2

```
% FINALLY USED VALUES SECTION %%%%%%
% Ok, next up, we are going to restrict most parameters to some ranges, and
% then pick parameter values at random from the set of remaining points.
% TX cat: 2.3 2.95
% RNase_Kd (index 6) ----> 15.59 15.73
% RNase_cat (index 7) ----> -0.2966 0.1031
% RNase (index 9) ----> 8.385 8.622
close all
paramIndices = [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13];
parRanges(paramIndices, :) = [...]
2.3 2.95; %1
8.6 8.95; %2
-10.1 -9.7; %3 delta atp (deg rate)
13 15; %4 pol Kd tet
-1 5 ; %5 pol term
15.59 15.73; %6 rnase KD
-0.2966 0.1031; %7rnase cat
0.7 2.2; %8 pol
8.385 8.622;%9 RNase
3.18 3.69; % 10 -- TLCat
-3 13.5;%RiboKd
2 3;% Ribo term
3 4.6 ];% Ribo
marray_cut = mcmc_cut(marray, paramIndices, flipud((parRanges(paramIndices, :))));
mcmc_plot(marray_cut(:, 1:end,ceil(end/4):end), parnames(), ...
'saveasmatlabfig', figsave, 'savejpeg', false, ...
'projdir', projdir, 'tstamp', tsToSave, 'extrafignamestring', 'BurnedIn');

CandidateParams = marray_cut(:, 1:100:end, end)
```



```
parRanges(paramIndices, :) = [...]
2.3 2.95; %1 tx cat
8.6 8.95; %2 tau
-10.1 -9.7; %3 delta atp (deg rate)
13 15; %4 pol Kd tet
-1 5 ; %5 pol term
15.59 15.73; %6 rnase KD
-0.2966 0.1031; %7rnase cat
0.7 2.2; %8 pol
8.385 8.622;%9 RNase
3.18 3.69; % 10 -- TLCat
-3 13.5;%RiboKd
2 3;% Ribo term
3 4.6 ];% Ribo
```



/Users/vipulsinghal/Dropbox/  
Documents/toolbox/  
txtlsim\_vsfork2017/mcmc\_simbio/  
projects/proj\_vnprl/  
simdata\_20190223\_024333\_1\_2/  
traj20190218\_135635\_1\_242MGa\_de  
GFP.jpg

[82ef659805d5d402b6644706528be893ccd8e964](#)

phase 1, mtet: (just ptet, ptet + tetR, ptet+tetR+atc)

```

+
% Thus, the 7 estimated parameters are:
3 % 'TXTL_PTET_RNAPbound_Kd' , 'est'
4 % 'TXTL_PTET_sequestration_Kd' , 'est'
5 % 'TXTL_PTET_sequestration_F' , 'est'
6 % 'TXTL_INDUCER_TETR_ATC_Kd' , 'est'
7 % 'TXTL_INDUCER_TETR_ATC_F' , 'est'
8 % 'TXTL_DIMER_tetR_Kd' , 'est'
9 % 'TXTL_DIMER_tetR_F' , 'est'

+
% 13x1 cell array
% ('TXL_cat') 1
% ('tau_atp') 3
% ('tau_ta') 5
% ('pol_tern') 21 % plac Kd NOT PTET Kd, the Ptet Kd gets estimated.
% ('RNase_Kd') 15
% ('RNase_cat') 30
% ('pol') 31
% ('RNase') 32
% ('TL_cat') 2
% ('Ribo_Kd') 6
% ('Ribo_tern') 28
% ('Ribo') 33

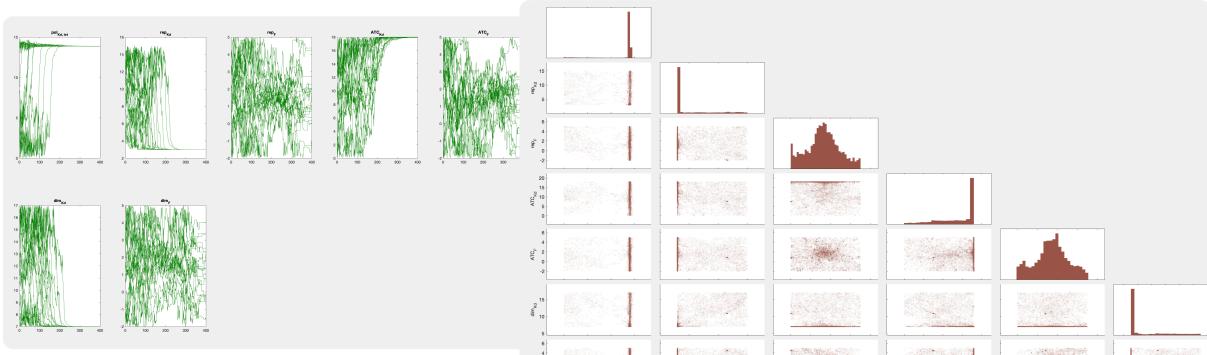
EstimatedParams =...
2.5234 2.4464 2.6231 2.5976 2.4658 2.4277 2.4896 2.6018 2.4391 2.5499 2.6991 2.4356
8.8054 8.9834 8.8097 8.8014 8.8483 8.8642 8.8394 8.8427 8.8616 8.7634 8.8622 8.7910
-18.819 -9.7873 -9.9376 -18.8948 -9.9856 -9.8889 -9.9100 -9.9631 -9.9827 -18.8348 -9.8782 -9.9538
13.7327 13.6474 13.8789 13.9325 13.7827 13.7665 13.7762 13.8681 13.8867 13.7211 14.4961 13.8706
2.8800 4.3598 0.0028 2.8127 3.5498 4.4008 4.1178 3.1338 0.3334 2.7831 1.8745 1.7856
15.6977 15.6349 15.7098 15.6858 15.6661 15.6339 15.7103 15.6193 15.6295 15.7294 15.6074 15.5958
0.8535 -0.2251 -0.1516 -0.0709 -0.2109 -0.1276 -0.0346 -0.1752 -0.0117 0.0436 -0.2481 -0.1603
1.1562 1.6167 1.4897 1.5206 1.6888 1.6259 1.6808 1.5196 1.7133 1.5597 1.4531 1.7096
8.3976 8.6141 8.6149 8.5123 8.5718 8.5146 8.4985 8.5494 8.3963 8.4382 8.6184 8.5097
3.6442 3.2731 3.2538 3.3823 3.2633 3.2387 3.4129 3.4928 3.3688 3.5169 3.3055
8.2565 0.0542 4.5196 -2.2731 -1.6399 -1.7370 -2.9377 0.6546 -1.7598 3.9814 6.7136 -0.3827
2.5533 2.8328 2.8292 2.7925 2.9282 2.8884 2.8659 2.9519 2.8087 2.7650 2.7130 2.9940
3.9583 4.1863 4.1261 4.0012 4.1922 3.9954 4.0318 3.7330 3.8616 4.1038 3.8526 3.8081;

ParamColumnToUse = 2;
paramVecToUse = EstimatedParams(:, ParamColumnToUse);
indicesMasterVectorEstimated = [1 3 5 21 23 15 30 31 32 2 6 28 33];
t1 = '20190428_071438_1_30039';
t2 = '20190428_071438_2_15465';
t3 = '20190428_155568_1_7732';
t4 = '20190428_155568_2_3003';
t5 = '20190428_155568_3_15465';
t6 = '20190428_155568_4_773';
t7 = '20190428_155568_5_309';
t8 = '20190428_155568_6_309';
t9 = '20190428_155568_7_77';
t10 = '20190428_155568_8_31';
t11 = '20190428_155568_9_31';

tstamp = {t1 t2 t3 t4 t5 t6 t7 t8 t9 t10 t11};
nterID = {1;2; 1:10 1:8 1:5 1:5 1:5 1:5 1:5 1:5 1:5 1:5 1:5 1:5};

tstamp = {t11 t2 t3 t4 t5 t6 t7 t8 t9 t10 t11};
nterID = {1;2; 1:10 1:8 1:5 1:5 1:5 1:5 1:5 1:5 1:5 1:5 1:5 1:5};

load([projdir '/models/_t11'] /fullVariableSet_ 't11.mat');
[m1, ...
'mmc_info', 'data_info', 'm1i', 'r1i'];
conclusions from case 2:
```



```

{'TXTL_PTET_RNAPbound_Kd' } {[ 0] } {[17]}
{'TXTL_PTET_sequestration_Kd'} {[ 3] } {[15]}
{'TXTL_PTET_sequestration_F' } {[ -2]} {[ 5]}
{'TXTL_INDUCER_TETR_ATC_Kd' } {[ 0]} {[18]}
{'TXTL_INDUCER_TETR_ATC_F' } {[ -2]} {[ 5]}
{'TXTL_DIMER_tetR_Kd' } {[ 7]} {[17]}
{'TXTL_DIMER_tetR_F' } {[ -2]} {[ 5]} ----- these were the parameter ranges for phase 1 estimated params. we can see from the graph above that

```

rep kd, atc kd and dim kd are hitting the boundaries, and need to be reestimated. we fix the rest, since they are either F rates or really tightly estimated kds:

```

prefixedParams2 = {...
7 'TXTL_PTET_RNAPbound_Kd' , exp(14)
12 'TXTL_PTET_sequestration_F' , exp(1.314)
17 'TXTL_INDUCER_TETR_ATC_F' , exp(1.577)
19 'TXTL_DIMER_tetR_F' , exp(1.447)};

```

These were found in phase 1, and fixed for phase 1b.

```

mtet_phase1_params = ...
{...
7 , 'TXTL_PTET_RNAPbound_Kd' , exp(14) , [exp(0) exp(25)]
11 , 'TXTL_PTET_sequestration_Kd' , exp(-1) , [exp(-10) exp(5)]
12 , 'TXTL_PTET_sequestration_F' , exp(1.314) , [exp(-2) exp(5)]}

```

```

16      ,      'TXTL_INDUCER_TETR_ATC_Kd'      ,      exp(-2)      ,      [exp(-15)      exp(5)]
17      ,      'TXTL_INDUCER_TETR_ATC_F'       ,      exp(1.577)    ,      [exp(-2)      exp(5)]
18      ,      'TXTL_DIMER_tetR_Kd'        ,      exp(-10)      ,      [exp(-20)      exp(-7)]
19      ,      'TXTL_DIMER_tetR_F'         ,      exp(1.447)    ,      [exp(-2)      exp(5)]...
};

The three highlighted parameters were the ones estimated in phase 1b, and those were the values found.

```

```

% 13x1 cell array
% ('TXL(cat)' ) 1
% ('tRNA(cat)' ) 3
% ('tRNA(atp)' ) 3
% ('sdeRNA(gp1)' ) 5
% ('pol_(Kd)' ) 21 % plac Kd NOT PTET Kd, the PtET Kd gets estimated.
% ('pol_(tern)' ) 23
% ('pol_(tetR)' ) 25
% ('tRNA_(cat)' ) 18
% ('pol' ) 31
% ('tRNA(atp)' ) 32
% ('sdeRNA(gp1)' ) 27
% ('Ribo_(Kd)' ) 6
% ('Ribo_(tern)' ) 28
% ('Ribo_(tetR)' ) 33
%
% 13x1 cell array
EstimatedParams =:, % 
- 2.5234 2.4664 ('TXL(cat)' ) 1
8.8854 8.9024 ('tRNA(atp)' ) 3
-10.0179 -9.2713 ('sdeRNA(gp1)' ) 5
1.1711 13.6101 ('pol_(Kd)' ) 21 % plac Kd NOT PTET Kd, the PtET Kd gets estimated.
2.0800 4.3598 ('pol_(tern)' ) 23
15.6977 15.6349 ('tRNAse_(Kd)' ) 15
8.0525 -8.4548 ('tRNAse_(cat)' ) 15
8.0525 8.1457 ('pol' ) 31
8.3976 8.6141 ('tRNA(atp)' ) 32
3.6442 3.2731 ('sdeRNA(gp1)' ) 2
8.2565 8.0542 ('Ribo_(Kd)' ) 3
2.5533 2.6328 ('Ribo_(tern)' ) 28
3.9983 4.3863 ('Ribo_(tetR)' ) 33
%
EstimatedParams =:, % 
ParamColumnTolse = 2
paramVecTolse = Est1;
indiceMasterVectorDf = -10.0179 -9.2713 -0.9376 -10.0048 -9.9856 -9.8889 -9.9100 -9.9531 -9.9827 -10.0348 -9.9782 -9.9538
+ 13.7327 13.6474 13.8789 13.9325 13.7827 13.7665 13.7762 13.8681 13.8867 13.7211 14.0961 13.8786
+ 2.5234 2.4664 2.6231 2.5976 2.4658 2.4277 2.4886 2.6018 2.4381 2.5499 2.6991 2.4356
+ 8.8854 8.9024 8.0807 8.8014 8.8483 8.8642 8.8394 8.8427 8.8616 8.7634 8.8621 8.7918
+ 0.0525 0.0525 0.0525 0.0525 0.0525 0.0525 0.0525 0.0525 0.0525 0.0525 0.0525 0.0525
+ 0.0525 -0.2251 -0.1516 -0.8789 -0.2109 -0.1276 -0.0340 -0.1752 -0.8117 0.0436 -0.2481 -0.1683
+ 1.5652 1.6167 1.4897 1.5286 1.6088 1.6259 1.6008 1.5196 1.7133 1.5597 1.4531 1.7096
+ 8.2565 8.6141 8.6141 8.5125 8.5118 8.5146 8.4965 8.5494 8.4957 8.4027 8.6184 8.5097
+ 3.6442 3.2731 3.2731 3.2658 3.2658 3.2658 3.1941 3.2087 3.1474 3.4028 3.3689 3.3803
+ 2.5533 2.6328 2.8292 2.7929 2.9282 2.8884 2.9859 2.9519 2.8887 2.7658 2.7136 2.9940
+ 3.9983 4.1863 4.1261 4.0812 4.1922 3.9954 4.0318 3.7338 3.8616 4.1838 3.8526 3.8881];
%
ParamColumnTolse = 2;
paramVecTolse = EstimatedParams(:, ParamColumnTolse);
+ indiceMasterVectorEstimated = [1 3 5 21 23 15 30 31 32 2 6 28 33];

```

/Users/vipulsinghal/Dropbox/Documents/toolbox/txtlsm\_vsfork2017/mcmc\_simbio/projects/proj\_ZSIFFL\_mtet/  
simdata\_20190420\_155505\_8\_31/cornerplot20190420\_155505\_8\_31AllWalkers.fig  
/Users/vipulsinghal/Dropbox/Documents/toolbox/txtlsm\_vsfork2017/mcmc\_simbio/projects/proj\_ZSIFFL\_mtet/  
simdata\_20190420\_155505\_8\_31/trace20190420\_155505\_8\_31AllWalkers.fig

mtet phase 1b is different from phase 1. the parameters estimated are

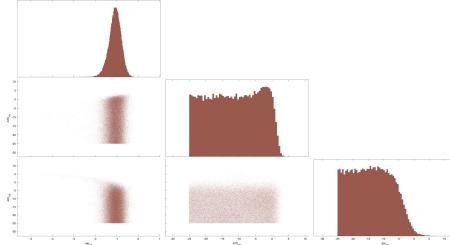
```
parnames = ...
[{'rep_{Kd}'}
 {'ATC_{Kd}'}
 {'dim_{Kd}'}
];
```

the files are sadly in the same folder: /Users/vipulsinghal/Dropbox/Documents/toolbox/txtlsm\_vsfork2017/mcmc\_simbio/projects/proj\_ZSIFFL\_mtet

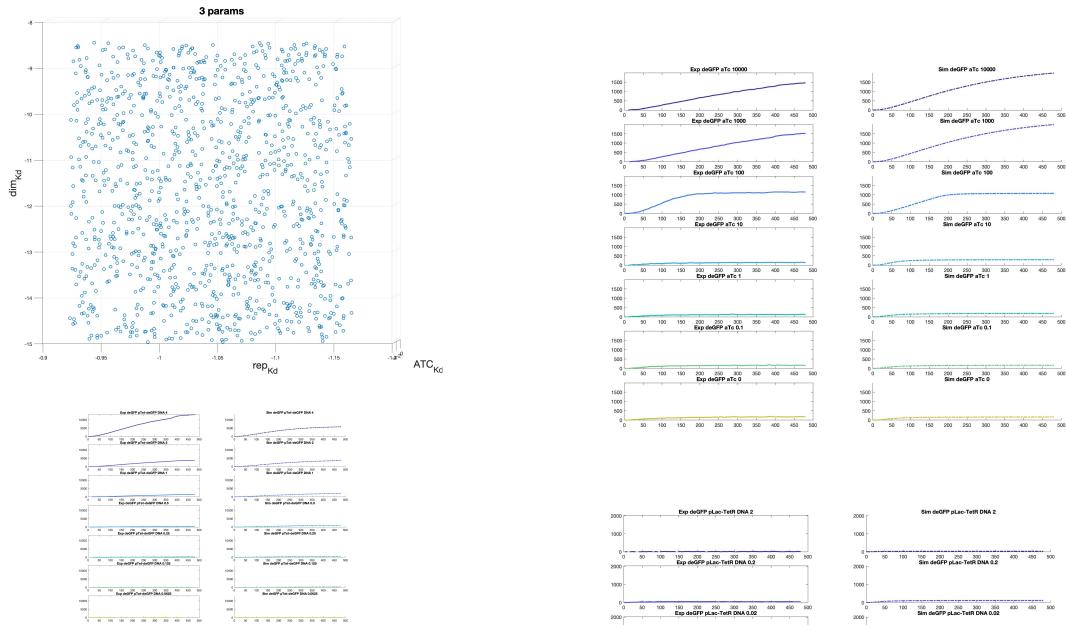
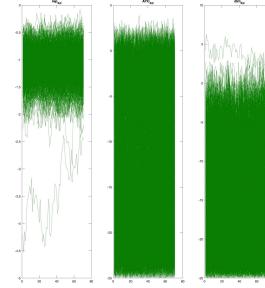
```
case 3
ts1 = '20190421_155749_1_773';
ts2 = '20190421_155749_2_309';
ts3 = '20190422_142534_1_773';
ts4 = '20190422_214228_1_773';
ts5 = '20190424_104801_1_773';

tstamp = {ts1 ts2 ts3 ts4 ts5};
niterID = (1:10 1:2 1:4 1:7 1:14);
load(['projdir' '/simdata' ts1 '/full_variable_set_ ts1 '.mat'], ...
'mi',...
'mcmc_info', 'data_info', 'mai', 'ri');

end
tsToSave = ts5;
mai.masterVector
```



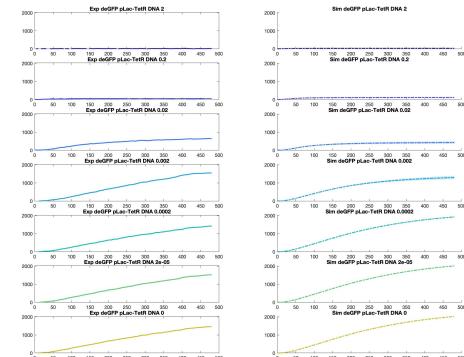
- 1, -2, -10 are the parameter values found here. see above.



/Users/vipulsinghal/Dropbox/Documents/toolbox/txtlsm\_vsfork2017/mcmc\_simbio/projects/proj\_ZSIFFL\_mtet/simdata\_20190424\_104801\_1\_773

### SCREEN RECORDING OF CARTESIAN PRODUCT.

/Users/vipulsinghal/Dropbox/Documents/toolbox/txtlsm\_vsfork2017/mcmc\_simbio/projects/proj\_ZSIFFL\_mtet/simdata\_20190424\_104801\_1\_773  
No\_cov\_fig\_cool.mov



## phase 2: add the plac constitutive production to the mix, and different set of parameters.

```
mcmc_info_ZSPTF_mix_phase2.m
% parameters of the master vector we fix and estimate
%
% The following params are the ones estimated from the last set of
% restrictions in the file analysis_vnprl_F2.m
%
% parameters
%
% 1x1 cell array
%
% {'Tx_(cat)' } 1
% {'TxL_(cat)' } 2
% {'Tdelta_(cat)' } 5
%
% {'pol_(Kd)' } 21 % plac Kd NOT PTET Kd, the PtET Kd gets estimated.
%
% {'RNaase_(cat)' } 1
% {'RNase_(cat)' } 15
% {'RNasec_(cat)' } 30
% {'RNaseL_(cat)' } 31
% {'RNase' } 32
% {'TL_(cat)' } 2
% {'RIBO_(cat)' } 6
% {'RIBO_(terms)' } 28
% {'Ribo' } 33
```

% The following were parameters estimated in vnprl\_F2, and were extracted
% to a master vector. These are the ones we need to fix to
% understand how they were picked. Need to document this before I forget.
EstimatedParams = ...
2.4277 2.5916 2.6231 2.5916 2.4656 2.4277 2.4896 2.4819 2.4301 2.5499 2.6991 2.4356
8.9824 8.8997 8.8914 8.8483 8.8942 8.8394 8.8427 8.7634 8.8621 8.7910
-10.0179 -9.7873 -9.9377 -10.8044 -9.9056 -9.8899 -9.5108 -9.9631 -9.9827 -10.8348 -9.8762 -9.9538
13.7320 13.7320 13.7320 13.7320 13.7320 13.7320 13.7320 13.7320 13.7320 13.7320 13.7320 13.7320
2.0880 4.3598 8.8928 2.8127 3.5498 4.4985 4.1178 3.1338 8.3334 2.7831 1.8745 1.7856
15.6977 15.6349 15.6893 15.6661 15.6339 15.7183 15.6193 15.6295 15.7294 15.6674 15.5958
0.4162 0.4162 0.4162 0.4162 0.4162 0.4162 0.4162 0.4162 0.4162 0.4162 0.4162 0.4162
1.5652 1.6167 1.4897 1.5296 1.6088 1.6259 1.6088 1.5196 1.7133 1.5597 1.4531 1.7896
8.3976 8.6141 8.6149 8.5123 8.5123 8.5146 8.4985 8.5494 8.3963 8.4382 8.6184 8.5897
3.0442 2.4242 2.4242 2.4242 2.4242 2.4242 2.4242 2.4242 2.4242 2.4242 2.4242 2.4242
0.2565 0.0542 4.5196 2.2731 -1.6399 -1.7570 -2.9377 0.6546 -1.7598 3.9814 6.7136 -0.3827
2.5533 2.8328 2.8292 2.7929 2.9282 2.8884 2.9559 2.9519 2.8887 2.7650 2.7138 2.9940
3.5983 4.1863 4.1261 4.0012 4.1922 3.9954 4.8318 3.7338 3.9816 4.1088 3.8526 3.8881;

```
ParamColumnTolUse = 2;
paramColUse = EstimatedParams(:, ParamColumnTolUse);
IndicesMasterVectorEstimated = [1 3 21 23 15 38 31 32 2 6 28 33];
```

- parameter ranges the estimation in phase 2 was carried out over.
- { 'TX\_elong\_glob' } { [ 0] } { [ 5] }
- { 'TL\_elong\_glob' } { [ 0] } { [ 6] }
- { 'AGTPdeg\_time' } { [ 6] } { [18] }
- { 'AGTPdeg\_ON' } { [ 0] } { [ 25] }
- { 'AGTPdeg\_Rate' } { [-10] } { [ 5] }
- { 'TXTL\_UTR\_UTR1\_Kd' } { [ 1] } { [ 10] }
- { 'TXTL\_PTET\_RNAPbound\_Kd' } { [ 1] } { [ 15] }
- { 'TXTL\_PTET\_RNAPbound\_F' } { [ 1] } { [ 15] }
- { 'TXTL\_PTET\_RNAF\_bound\_Kd' } { [ 1] } { [ 15] }
- { 'TXTL\_PTET\_RNAF\_bound\_2\_Kd' } { [ 1] } { [ 15] }
- { 'TXTL\_PTET\_sequestration\_Kd' } { [ 1] } { [ 15] }
- { 'TXTL\_PTET\_sequestration\_F' } { [ 1] } { [ 15] }
- { 'TL\_AA\_Kd' } { [ 1] } { [ 15] }
- { 'TL\_AGP\_Kd' } { [ 1] } { [ 15] }
- { 'TXTL\_RNAdeg\_Kd' } { [ 1] } { [ 15] }
- { 'TXTL\_INDUCER\_TETR\_ATC\_Kd' } { [ 1] } { [ 15] }
- { 'TXTL\_INDUCER\_TETR\_ATC\_F' } { [ 1] } { [ 15] }
- { 'TXTL\_DIMER\_tetR\_Kd' } { [ 1] } { [ 15] }
- { 'TXTL\_DIMER\_tetR\_F' } { [ 1] } { [ 15] }
- { 'TXTL\_UTR\_UTR1\_F' } { [ 1] } { [ 15] }
- { 'TXTL\_PTET\_RNAPbound\_Kd' } { [ 1] } { [ 15] }
- { 'TXTL\_PLAC\_RNAPbound\_F' } { [ 1] } { [ 15] }
- { 'TXTL\_RNAPBOUND\_TERMINATION\_RATE' } { [ 1] } { [ 15] }
- { 'TXTL\_NTP\_RNAP\_1\_F' } { [ 1] } { [ 15] }
- { 'TXTL\_NTP\_RNAP\_2\_F' } { [ 1] } { [ 15] }
- { 'TL\_AA\_F' } { [ 1] } { [ 15] }
- { 'TL\_AGP\_F' } { [ 1] } { [ 15] }
- { 'TXTL\_RIBOBOUND\_TERMINATION\_RATE' } { [ 1] } { [ 15] }
- { 'TXTL\_RNAdeg\_F' } { [ 1] } { [ 15] }
- { 'TXTL\_RNAdeg\_Kc' } { [ 1] } { [ 15] }
- { 'RNAP' } { [ 1] } { [ 15] }
- { 'RNase' } { [ 1] } { [ 12] }
- { 'Ribo' } { [ 1] } { [ 12] }

```
activeNames = {..., % param name, nominal value, range of parameters for uniform prior,
'TX_elong_glob' , exp(2.6), [exp(0) exp(5)] %3 from est params above
'TL_elong_glob' , exp(3.5), [exp(0) exp(6)] %2 from est params above
'AGTPdeg_time' , exp(8.8), [exp(6) exp(18)] %3 from est params above
'AGTPreg_ON' , exp(-3.9), [exp(-6) exp(-1)] %4 fixed in mcmc_info_vnprl_F2
'AGTPdeg_Rate' , exp(-9.9), [exp(-13) exp(-7)] %5 from est params above
'TXTL_UTR_UTR1_Kd' , exp(11), [exp(-3) exp(15)] %6 from est params above
'TXTL_PTET_RNAPbound_Kd' , exp(14), [exp(0) exp(17)] %7 TO BE ESTIMATED HERE
'TXTL_PTET_RNAPbound_F' , exp(1.5), [exp(0) exp(4)] %8 fixed in mcmc_info_vnprl_F2
'TXTL_PTET_RNAF_bound_Kd' , exp(2.9), [exp(0) exp(5)] %9 fixed in mcmc_info_vnprl_F2
'TXTL_PTET_RNAF_bound_2_Kd' , exp(14), [exp(10) exp(20)] %10 fixed in mcmc_info_vnprl_F2
'TXTL_PTET_sequestration_Kd' , exp(12), [exp(3) exp(15)] %11 TO BE ESTIMATED HERE
'TXTL_PTET_sequestration_F' , exp(1.5), [exp(-2) exp(5)] %12 TO BE ESTIMATED HERE
'TL_AA_Kd' , exp(6.6), [exp(3) exp(10)] %13 fixed in mcmc_info_vnprl_F2
'TL_AGP_Kd' , exp(14.5), [exp(10) exp(18)] %14 fixed in mcmc_info_vnprl_F2
'TXTL_RNAdeg_Kd' , exp(15.2), [exp(7) exp(17)] %15 from est params above
'TXTL_INDUCER_TETR_ATC_Kd' , exp(13), [exp(0) exp(18)] %16 TO BE ESTIMATED HERE
'TXTL_INDUCER_TETR_ATC_F' , exp(2.6), [exp(-2) exp(5)] %17 TO BE ESTIMATED HERE
'TXTL_DIMER_tetR_Kd' , exp(13), [exp(7) exp(17)] %18 TO BE ESTIMATED HERE
'TXTL_DIMER_tetR_F' , exp(12), [exp(-2) exp(5)] %19 TO BE ESTIMATED HERE
'TXTL_UTR_UTR1_F' , exp(-1.2), [exp(-4) exp(2)] %20 fixed in mcmc_info_vnprl_F2
'TXTL_PTET_RNAPbound_Kd' , exp(13.8), [exp(5) exp(17)] %21 from est params above
'TXTL_PLAC_RNAPbound_F' , exp(2.6), [exp(-2) exp(5)] %22 fixed in mcmc_info_vnprl_F2
'TXTL_RNAPBOUND_TERMINATION_RATE' , exp(1.8), [exp(-3) exp(6)] %23 from est params above
'TXTL_NTP_RNAP_1_F' , exp(0), [exp(-2) exp(3)] %24 fixed in mcmc_info_vnprl_F2
'TXTL_NTP_RNAP_2_F' , exp(0), [exp(-2) exp(3)] %25 fixed in mcmc_info_vnprl_F2
'TL_AA_F' , exp(-0.3), [exp(-3) exp(3)] %26 fixed in mcmc_info_vnprl_F2
'TL_AGP_F' , exp(-1.2), [exp(-4) exp(2)] %27 fixed in mcmc_info_vnprl_F2
'TXTL_RIBOBOUND_TERMINATION_RATE' , exp(2.3), [exp(0) exp(5)] %28 from est params above
'TXTL_RNAdeg_F' , exp(0), [exp(-3) exp(3)] %29 fixed in mcmc_info_vnprl_F2
'TXTL_RNAdeg_Kc' , exp(-0.45), [exp(-5) exp(3)] %30 from est params above
'RNAP' , exp(1.4419), [exp(-1) exp(15)] %31 31% from est params above
'RNase' , exp(8.5), [exp(5) exp(12)] %32 from est params above
'Ribo' , exp(3.75), [exp(1) exp(12)] %33 from est params above
'TXTL_PROT_deGFP_MATURATION' , exp(-6.07), [exp(-9) exp(-3)] %34 fixed in mcmc_info_vnprl_F2
```

```
% Set the master vector values that are set from the values estimated in "vnprl_F2"
activeNames(indicesMasterVectorEstimated, 2) = num2cell(exp(paramVecToUse));
```

```
preFixedParams = {...
4 'AGTPreg_ON' , exp( -3.9120)
34 'TXTL_PROT_deGFP_MATURATION' , exp( -6.0748)
8 'TXTL_PTET_RNAPbound_F' , exp( 1.5000)
9 'TXTL_NTP_RNAP_1_Kd' , exp( 2.9459)
10 'TXTL_NTP_RNAP_2_Kd' , exp( 13.9970)
13 'TL_AA_Kd' , exp( 6.5566)
14 'TL_AGP_Kd' , exp( 14.5090)
20 'TXTL_UTR_UTR1_F' , exp( -0.2000)
22 'TXTL_PLAC_RNAPbound_F' , exp( 1.5000)
24 'TXTL_NTP_RNAP_1_F' , exp( 0)
25 'TXTL_NTP_RNAP_2_F' , exp( 0)
26 'TL_AA_F' , exp( -0.3000)
27 'TL_AGP_F' , exp( -1.2000)
29 'TXTL_RNAdeg_F' , exp( 0); % checked and verified.
```

```
mtet_phase1_params = ...
{...
7 , 'TXTL_PTET_RNAPbound_Kd' , exp(14) , [exp(0) exp(25)]
11 , 'TXTL_PTET_sequestration_Kd' , exp(-1) , [exp(-10) exp(5)]
12 , 'TXTL_PTET_sequestration_F' , exp(1.314) , [exp(-2) exp(5)]
16 , 'TXTL_INDUCER_TETR_ATC_Kd' , exp(-2) , [exp(-15) exp(5)]
17 , 'TXTL_INDUCER_TETR_ATC_F' , exp(1.577) , [exp(-2) exp(5)]
18 , 'TXTL_DIMER_tetR_Kd' , exp(-10) , [exp(-20) exp(-7)]
19 , 'TXTL_DIMER_tetR_F' , exp(1.447) , [exp(-2) exp(5)]...}
```

```

activeNames(cell2mat(mttet_phase1_params(:,1)),2) = mttet_phase1_params(:,3);
activeNames(cell2mat(mttet_phase1_params(:,1)),3) = mttet_phase1_params(:,4);
% Thus, the 10 estimated parameters are:

% 'TX_elong_glob' , exp(2.6), [exp(0) exp(5)] %1 % from est params above
% 'TL_elong_glob' , exp(3.5), [exp(0) exp(6)] %2 % from est params above
% 'AGTdeg_time' , exp(8.8), [exp(6) exp(11)] %3 % from est params above
% 'TXTL_Pdeg_time' , exp(14), [exp(0) exp(17)] %7 % TO BE ESTIMATED HERE
% 'TXTL_PTEI_sequestration_Kd' , exp(12), [exp(3) exp(15)] %11 % TO BE ESTIMATED HERE
% 'TXTL_INDUCER_TETR_ATC_Kd' , exp(13), [exp(0) exp(18)] %16 % TO BE ESTIMATED HERE
% 'TXTL_PLAC_RNAPbound_Kd' , exp(13.8), [exp(5) exp(17)] %21 from est params above
% 'RNAP' , exp(1.4419), [exp(-1) exp(4)] %31 31% from est params above
% 'RNase' , exp(8.5), [exp(5) exp(10)] %32 from est params above
% 'Ribo' , exp(3.75), [exp(1) exp(6)] %33 % from est params above

```

```

estParamsIX = [1 2 3 7 11 16 21 31 32 33]';
estParams = activeNames(estParamsIX,1);
activeNames
% skipping AGTPdeo rate. AGTPdeo ON. TXTL PROT deGFP MATURATION

```

```

tsIDtouse = 4;
plotflag = true;
switch tsIDtouse

case 1
    ts1 = '20190427_170334_1_2058';
    ts2 = '20190427_170334_2_1029';

    tstamp = {ts1 ts2};
    niterID = {1:10 1:3};
    load(projdir '/simdata/' ts1 '/full_variable_set_' ts1 '.mat', ...
        'm1',...
        'mcmc_info', 'data_info', 'mai', 'ri');

case 2
    ts1 = '20190428_142033_1_2058';
    ts2 = '20190428_142033_2_1029';
    ts3 = '20190429_083138_1_1029';
    ts4 = '20190429_200219_1_1029';
    ts5 = '20190429_200219_2_412';
    ts6 = '20190430_141254_1_412';
    ts7 = '20190430_141254_2_206';
    ts8 = '20190501_042800_1_1029';
    ts9 = '20190501_105714_1_412';
    ts10 = '20190502_105714_1_412';
    ts11 = '20190503_073640_1_412';
    ts12 = '20190503_113414_1_412';
    ts13 = '20190503_170440_1_412';
    ts14 = '20190504_155250_1_412';
    tstamp = {ts1 ts2 ts3 ts4 ts5 ts6 ts7 ts8 ts9 ts10 ts11 ts12 ts13 ts14};
    niterID = {1:10 1:2 1:4 1:5 1:3 1:5 1:5 1:4 1:8 1:11 1 1 1 11 13};
    load(projdir '/simdata/' ts1 '/full_variable_set_' ts1 '.mat', ...
        'm1',...
        'mcmc_info', 'data_info', 'mai', 'ri');

end
tsToSave = ts14;
mai.masterVector

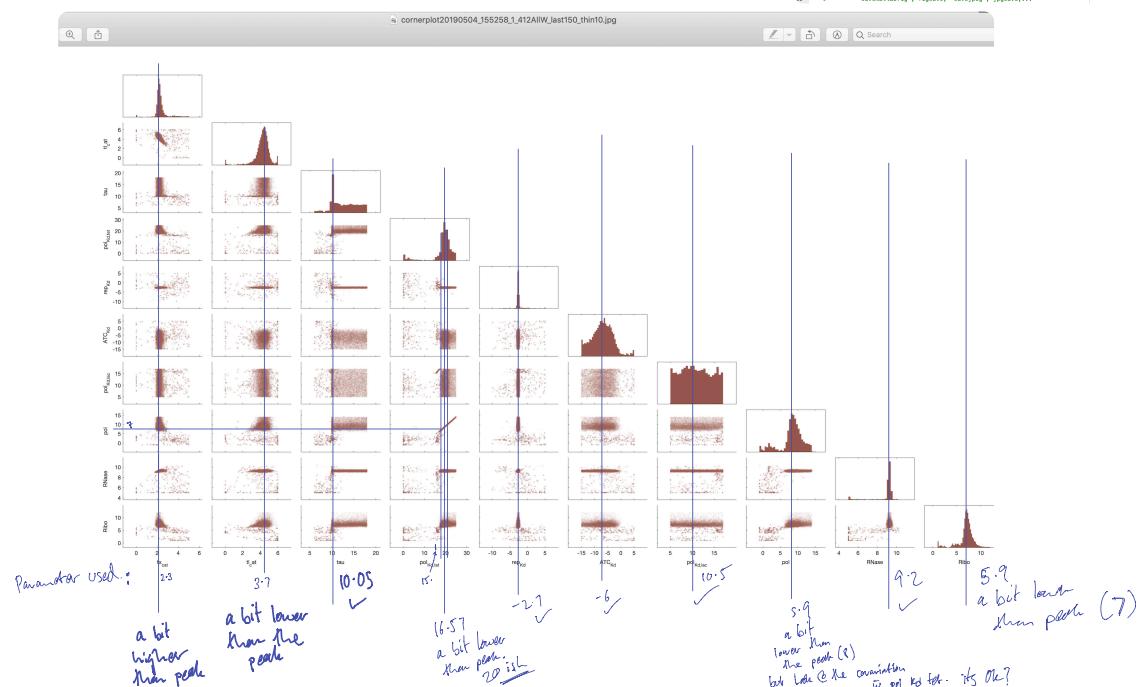
```

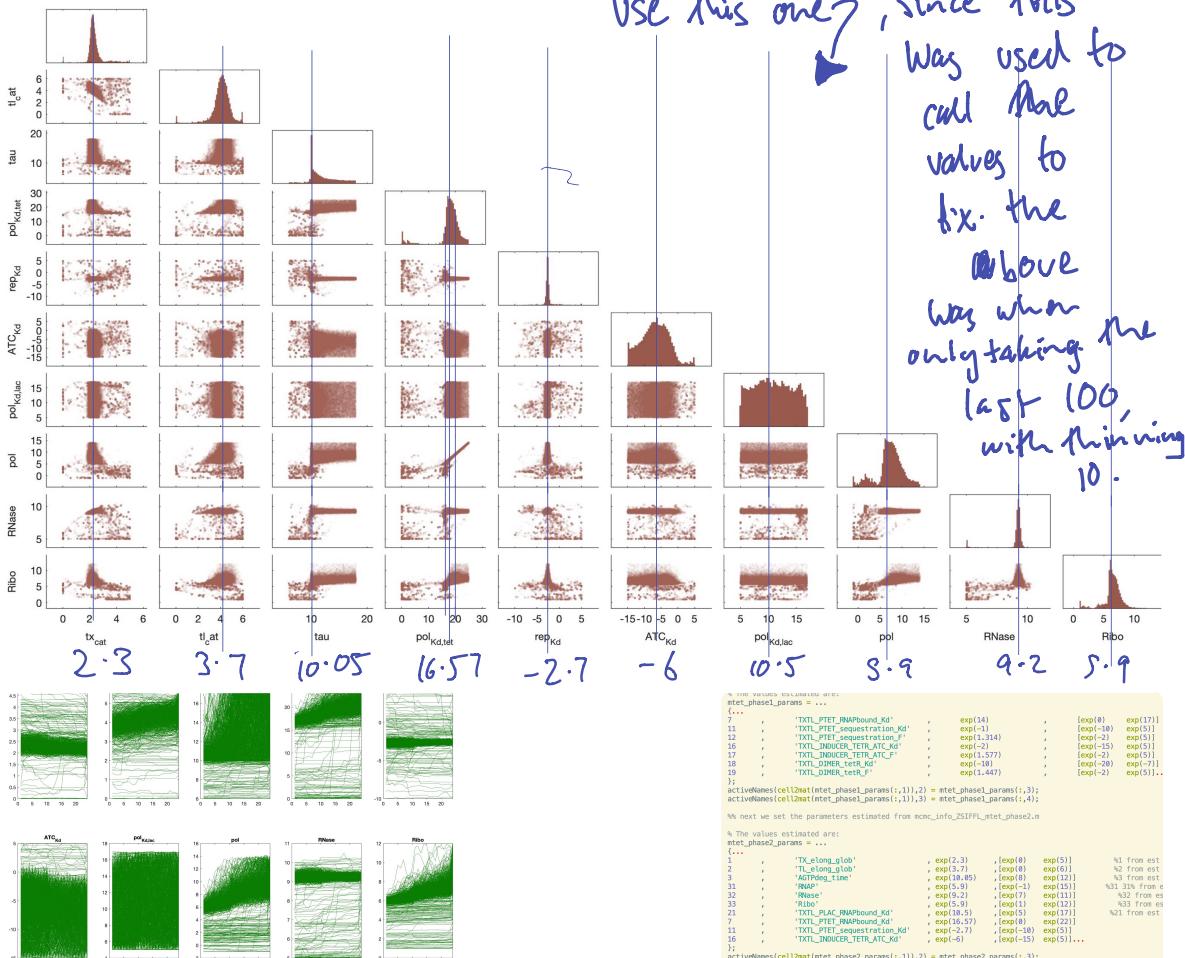
1aa864160f23c1ef7b89ea1412cee7d9006aeaab

```

91 % {'Kobs'}
92 % if plotflag
93 %    mode_plantmatrix, l1end, l1end-1800)1000, paramset());
94 %    mode_plantmatrix, l1gave, l1gave); jpsave, ...
95 %    'projdir', projdir, 'l1name', ts1, 'l1rungetting', 'AllW_l1ts1_main');
96 %    'wcc_plantmatrix1, l1end, l1end, paramset(), ...
97 %    l1gave, l1gave); jpsave, ...
98 %    'wcc_plantmatrix1, l1gave, l1gave); jpsave, ...

```





```
% time variables in seconds
met_phase1_params = ...
{...
    'TXTL_PET_PMAPbound_Kd' , exp(14) , [exp(8) exp(17)] ...
    'TXTL_PET_sequestration_Kd' , exp(-1) , [exp(-18) exp(5)] ...
    'TXTL_PET_sequestration_F' , exp(1.214) , [exp(-2) exp(5)] ...
    'TXTL_INDUCER_TETR_ATC_F' , exp(1.577) , [exp(-2) exp(5)] ...
    'TXTL_INDUCER_TETR_ATC_Kd' , exp(1.577) , [exp(-2) exp(5)] ...
    'TXTL_DIMER_ExtF' , exp(1.447) , [exp(-2) exp(5)] ...
};

activeNames(cell12m(atet_phase1_params(:,1),2)) = atet_phase1_params(:,3);
activeNames(cell12m(atet_phase1_params(:,1),3)) = atet_phase1_params(:,4);

% next we set the parameters estimated from mcmc_info_ZSIFFL_atet_phase1.n
% The values estimated are:
met_phase2_params = ...
{...
    'TXL_elong_glob' , exp(2.0) , [exp(8) exp(5)] ...
    'TL_elong_glob' , exp(3.7) , [exp(8) exp(6)] ...
    'ActProg_time' , exp(18.85) , [exp(8) exp(12)] ...
    'RNase' , exp(9.2) , [exp(7) exp(11)] ...
    'RNase' , exp(9.2) , [exp(7) exp(11)] ...
    'TXTL_PLAC_PMAPbound_Kd' , exp(18.5) , [exp(8) exp(17)] ...
    'TXTL_PET_PMAPbound_Kd' , exp(16.577) , [exp(8) exp(22)] ...
    'TXTL_INDUCER_TETR_ATC_F' , exp(-8) , [exp(-15) exp(5)] ...
    'TXTL_INDUCER_TETR_ATC_Kd' , exp(-8) , [exp(-15) exp(5)] ...
};

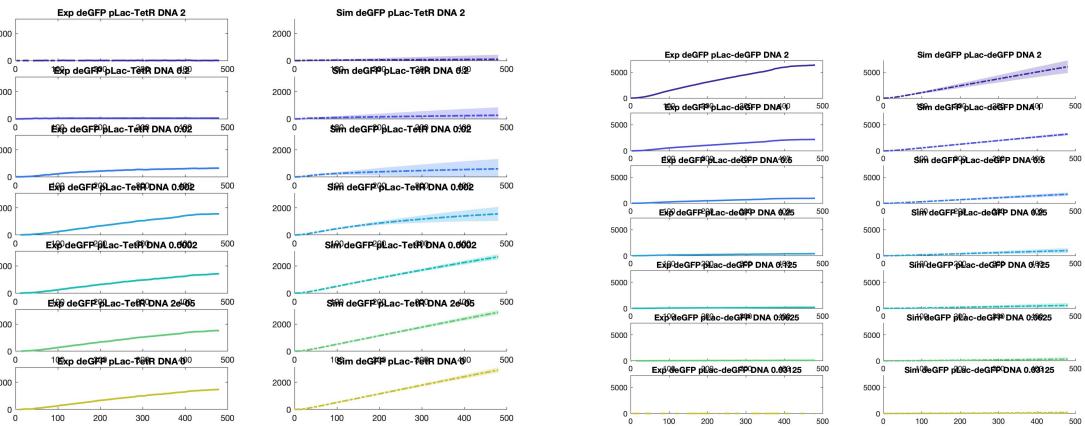
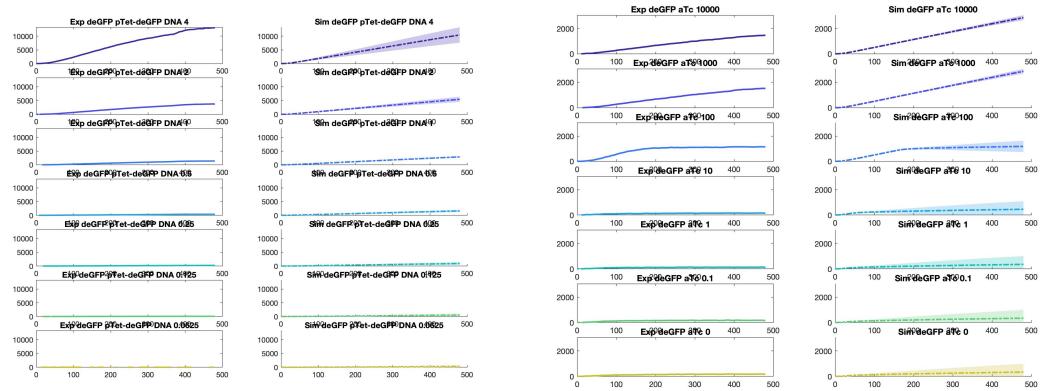
activeNames(cell12m(atet_phase2_params(:,1),2)) = atet_phase2_params(:,3);
activeNames(cell12m(atet_phase2_params(:,1),3)) = atet_phase2_params(:,4);

% we also set the forward rate parameters, since those should not matter much, and any value around 1 is
% the F rate parameters just set the timescale.
atet_phase2_params = ...
{...
    'TXTL_INDUCER_LASR_AHL_F' , exp(0) , [exp(-3) exp(5)] ...
    'TXTL_PLAS_RNAPbound_F' , exp(0) , [exp(-3) exp(5)] ...
    'TXTL_PLAS_RNAPbound_D' , exp(0) , [exp(-3) exp(5)] ...
    'TXTL_PLAS_TRANS_F' , exp(0) , [exp(-3) exp(5)] ...
};

activeNames(cell12m(atet_phase2_params(:,1),2)) = atet_phase2_params(:,3);
activeNames(cell12m(atet_phase2_params(:,1),3)) = atet_phase2_params(:,4);
```

/Users/vipulsinghal/Dropbox/Documents/toolbox/txtlsm\_vsfork2017/mcmc\_simbio/projects/proj\_ZSIFFL\_mtet\_phase2/simdata\_20190504\_155258\_1\_412

This went through a few iterations of parameter range expansion. commits  
[da77c5446bd97c422207b3d5854fd70206ce6c8](#) to [27cb38b91e8b96547a4ee9e91f5188a26bba0800](#)



```

case 1
ts1 = '28190001_070000_1_180';
ts2 = '28190001_123454_1_180';
ts3 = '28190001_123454_2_180';
ts4 = '28190001_123454_3_180';
ts5 = '28190001_128418_1_180';

tstamp = [ts1 ts2 ts3 ts4 ts5];
nterID = {1 15 15 1 12 12};
loadFile = 'simdata_1.tsl' 'full_variable_set_1.ts1'.mat'; ...
'nter_id',...
'mcmc_info', 'data_info', 'mai', 'ri1';

% The values estimated are:
mtet_phasel_params = ...
{...
7 , 'TXTL_PTET_RNAPbound_Kd' , exp(14) , [exp(0) exp(5)] %1 from est
11 , 'TXTL_PTET_sequestration_Kd' , exp(-1) , [exp(-10) exp(5)] %2 from est
12 , 'TXTL_PTET_sequestration_F' , exp(1.314) , [exp(-2) exp(5)] %3 from est
16 , 'TXTL_DIMER_tetR_AHL_Kd' , exp(0.001) , [exp(0) exp(5)] %31 31% from est
17 , 'TXTL_INDUCER_TETR_ATC_F' , exp(1.577) , [exp(-2) exp(5)] %33 from est
18 , 'TXTL_DIMER_tetKd' , exp(-10) , [exp(-20) exp(-7)] %33 from est
19 , 'TXTL_DIMER_tetF' , exp(1.447) , [exp(-2) exp(5)]..

activeNames(cell2mat(mtet_phase1_params(:,1)),2) = mtet_phase1_params(:,3);
activeNames(cell2mat(mtet_phase1_params(:,1)),3) = mtet_phase1_params(:,4);

% next we set the parameters estimated from mcmc_info_ZSIFFL_mtet_phase2.m
% The values estimated are:
mtet_phase2_params = ...
{...
1 , 'RIBO_elong_glob' , exp(2.3) , [exp(0) exp(5)] %1 from est
2 , 'RIBO_elong_glob' , exp(3.7) , [exp(0) exp(6)] %2 from est
3 , 'AGTPdeq_time' , exp(10.05) , [exp(0) exp(12)] %3 from est
31 , 'RNAP' , exp(5.9) , [exp(-1) exp(15)] %31 31% from est
32 , 'RIBO' , exp(0.001) , [exp(0) exp(5)] %33 from est
33 , 'RIBO' , exp(5.9) , [exp(1) exp(12)] %33 from est
21 , 'TXTL_PTET_RNAPbound_Kd' , exp(10.57) , [exp(0) exp(17)] %21 from est
7 , 'TXTL_PTET_RNAPbound_F' , exp(16.57) , [exp(0) exp(22)] %21 from est
11 , 'TXTL_PTET_sequestration_Kd' , exp(-2.7) , [exp(-10) exp(5)] %21 from est
16 , 'TXTL_INDUCER_TETR_ATC_Kd' , exp(-6) , [exp(-15) exp(5)]..

activeNames(cell2mat(mtet_phase2_params(:,1)),2) = mtet_phase2_params(:,3);
activeNames(cell2mat(mtet_phase2_params(:,1)),3) = mtet_phase2_params(:,4);

% we also set the forward rate parameters, since those should not matter much, and any value around 1 is
% the f_rate parameter. we just set the timescale.
mtet_phase2_params = ...
{...
36 , 'TXTL_INDUCER_LASR_AHL_F' , exp(0) , [exp(-3) exp(5)] %1 from est
38 , 'TXTL_PLAS_RNAPbound_F' , exp(0) , [exp(0) exp(5)] %2 from est
41 , 'TXTL_PLAS_TFBIND_R' , exp(0) , [exp(0) exp(5)] %3 from est
42 , 'TXTL_PLAS_TFBIND_F' , exp(0) , [exp(-3) exp(5)]..

activeNames(cell2mat(mtet_phase2_params(:,1)),2) = mtet_phase2_params(:,3);
activeNames(cell2mat(mtet_phase2_params(:,1)),3) = mtet_phase2_params(:,4);

% Set the master vector values that are set from the values estimated in 'vn
activeNames(indicesMasterVectorEstimated, 2) = num2cell(exp(paramVecToUse));

```

```

% Set the master vector values that were already fixed in 'vnprl_F2'
prefixedParams = {...
4 , 'AGTPdeq_time' , ...
34 , 'TXTL_PTET_deGFP_MATURATION' , exp(-3.9120) %1 from est
, exp(-6.0748) %2 from est
8 , 'TXTL_PTET_RNAPbound_F' , exp(1.5000) %3 from est
9 , 'TXTL_NTP_RNAP_1_Kd' , exp(2.9459) %31 31% from est
10 , 'TXTL_NTP_RNAP_2_Kd' , exp(13.9970) %33 from est
13 , 'TL_AA_Kd' , exp(6.5566) %33 from est
14 , 'TL_AGP_Kd' , exp(14.5090) %21 from est
20 , 'TXTL_UTR_UTR1_F' , exp(-0.2000) %21 from est
22 , 'TXTL_PLAC_RNAPbound_F' , exp(1.5000) %21 from est
24 , 'TXTL_NTP_RNAP_1_F' , exp( 0) %21 from est
25 , 'TXTL_NTP_RNAP_2_F' , exp( 0) %21 from est
26 , 'TL_AA_F' , exp(-0.3000) %21 from est
27 , 'TL_AGP_F' , exp(-1.2000) %21 from est
29 , 'TXTL_NNAdeg_F' , exp( 0)); % checked and ve

```

```

paramnames = ...
{...
{'pol_{(Kd,tet)}'}
{'pol_{(Kd,lac)}'}
{'pol'}
{'Ribo'}
{'3OC12_{(Kd)}'}
{'3OC12_{(F)}'}
{'pol_{(Kd,las)}'}
{'pol_{(F,las)}'}
{'plas_{(tf, Kd)}'}
{'plas-pol_{(tf, Kd)}'}
{'plas-pol_{(tf, F)}'}
{'plas_{(tf, F)}'}
};

% activeNames(estParams)

```

Reaction: '[protein lasR] + OC12HSL <-> [OC12HSL:protein lasR]'  
 ReactionRate: [TXTL\\_INDUCER\\_LASR\\_AHL\\_F](#)[protein lasR]\*OC12HSL - TXTL\_INDUCER\_LASR\_AHL\_R\*[OC12HSL:protein lasR]

Reaction: '[DNA plas--utr1--deGFP] + RNAP <-> [RNAP:DNA plas--utr1--deGFP]'  
 ReactionRate: [TXTL\\_PLAS\\_RNAPbound\\_F](#)\*[DNA plas--utr1--deGFP]\*RNAP - TXTL\_PLAS\_RNAPbound\_R\*[RNAP:DNA plas--utr1--deGFP]

Reaction: '[DNA plas--utr1--deGFP] + [OC12HSL:protein lasR] <-> [DNA plas--utr1--deGFP:OC12HSL:protein lasR]'  
 ReactionRate: [TXTL\\_PLAS\\_TFBIND\\_F](#)\*[DNA plas--utr1--deGFP]\*[OC12HSL:protein lasR] - TXTL\_PLAS\_TFBIND\_R\*[DNA plas--utr1--deGFP:OC12HSL:protein lasR]

Reaction: '[DNA plas--utr1--deGFP:OC12HSL:protein lasR] + RNAP <-> [RNAP:DNA plas--utr1--deGFP:OC12HSL:protein lasR]'  
 ReactionRate: [TXTL\\_PLAS\\_TFRNAPbound\\_F](#)\*[DNA plas--utr1--deGFP:OC12HSL:protein lasR]\*RNAP - TXTL\_PLAS\_TFRNAPbound\_R\*[RNAP:DNA plas--utr1--deGFP:OC12HSL:protein lasR]

Reaction: '[RNAP:DNA plas--utr1--deGFP] + [OC12HSL:protein lasR] <-> [RNAP:DNA plas--utr1--deGFP:OC12HSL:protein lasR]'  
 ReactionRate: [TXTL\\_PLAS\\_TFBIND\\_F](#)\*[RNAP:DNA plas--utr1--deGFP]\*[OC12HSL:protein lasR] - TXTL\_PLAS\_TFBIND\_R\*[RNAP:DNA plas--utr1--deGFP:OC12HSL:protein lasR]

why the hell are these named the same way??? i think it does not matter,  
 since i update activeNames with them, but still, this is just an error  
 waiting to happen.

% we also set the forward rate parameters, since those should not matter much, and any value around 1 is  
 the f\_rate parameter. we just set the timescale.

mtet\_phase2\_params = ...

{...
36 , 'TXTL\_INDUCER\_LASR\_AHL\_F' , exp(0) , [exp(-3) exp(5)] %1 from est
38 , 'TXTL\_PLAS\_RNAPbound\_F' , exp(0) , [exp(0) exp(5)] %2 from est
41 , 'TXTL\_PLAS\_TFBIND\_R' , exp(0) , [exp(0) exp(5)] %3 from est
42 , 'TXTL\_PLAS\_TFBIND\_F' , exp(0) , [exp(-3) exp(5)]..

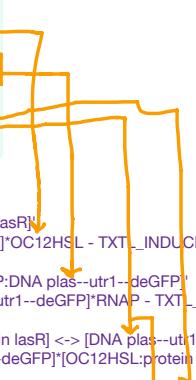
activeNames(cell2mat(mtet\_phase2\_params(:,1)),2) = mtet\_phase2\_params(:,3);
activeNames(cell2mat(mtet\_phase2\_params(:,1)),3) = mtet\_phase2\_params(:,4);

% Set the master vector values that are set from the values estimated in 'vn

activeNames(indicesMasterVectorEstimated, 2) = num2cell(exp(paramVecToUse));

Dont know this was ever  
 estimated. We fixed  
 from the moment  
 they were introduced

WAS THIS THE  
 ORIGINAL  
 TRAINING  
 FULL ???



Overall summary of what was estimated where and to what values.

- training full, before May 6 commit.

```

ans =
12x3 cell array
    ('TXTL_PTET_RNAPbound_Kd') {[1.5713e+07]} {1x2 double}
    ('TXTL_PLAC_RNAPbound_Kd') {[3.6316e+04]} {1x2 double}
    ('RNAP') {[365.0375]} {1x2 double}
    ('Ribo') {[365.0375]} {1x2 double}
    ('TXTL_INDUCER_LASR_AHL_Kd') {[0.1353]} {1x2 double}
    ('TXTL_INDUCER_LASR_AHL_F') {[3.6693]} {1x2 double}
    ('TXTL_PLAS_RNAPbound_Kd') {[0.1353]} {1x2 double}
    ('TXTL_PLAS_RNAPbound_F') {[3.6693]} {1x2 double}
    ('TXTL_PLAS_TFBIND_Kd') {[0.1353]} {1x2 double}
    ('TXTL_PLAS_TFRNAPbound_Kd') {[7.3891]} {1x2 double}
    ('TXTL_PLAS_TFRNAPbound_F') {[3.6693]} {1x2 double}
    ('TXTL_PLAS_TFBIND_F') {[3.6693]} {1x2 double}

f2 >> |

training all B
training all C
training all D
in addition to those listed in C.
Fixed in E?
or just in E?

estParamsIX = [23 28 31 33 35 37 39 40];
estParams = activeNames(estParamsIX,1)

estParams =
1x1 cell array
    ('TX_elong_glob')
    ('TL_elong_glob')
    ('TXTL_PTET_RNAPbound_Kd')
    ('TXTL_PTET_sequestration_Kd')
    ('TXTL_RIBOBOUND_TERMINATION_RATE')
    ('TXTL_RIBOBOUND_TERMINATION_RATE')
    ('RNAP')
    ('Ribo')
    ('TXTL_INDUCER_LASR_AHL_Kd')
    ('TXTL_INDUCER_LASR_AHL_F')
    ('TXTL_PLAS_TFBIND_Kd')
    ('TXTL_PLAS_TFRNAPbound_Kd')
    ('TXTL_PLAS_TFBIND_F')

estParamsIX = [1 2 7 11 16 21 23 28 31 33 35 37 39 40];
estParams = activeNames(estParamsIX,1)

estParams =
1x1 cell array
    ('TX_elong_glob')
    ('TL_elong_glob')
    ('TXTL_PTET_RNAPbound_Kd')
    ('TXTL_PTET_sequestration_Kd')
    ('TXTL_RIBOBOUND_TERMINATION_RATE')
    ('TXTL_RIBOBOUND_TERMINATION_RATE')
    ('RNAP')
    ('Ribo')
    ('TXTL_INDUCER_LASR_AHL_Kd')
    ('TXTL_INDUCER_LASR_AHL_F')
    ('TXTL_PLAS_RNAPbound_Kd')
    ('TXTL_PLAS_TFBIND_Kd')
    ('TXTL_PLAS_TFRNAPbound_Kd')

Fitting did not work
Don't need to put into paper.

training all E.

mte_phase2_params = ...
(...
36     , 'TXTL_PTET_RNAPbound_Kd' , exp(0) , [exp(-3) exp(5)]
38     , 'TXTL_PLAS_RNAPbound_F' , exp(0) , [exp(-3) exp(5)]
39     , 'TXTL_PLAS_RNAPbound_Kd' , exp(0) , [exp(-3) exp(5)]
40     , 'TXTL_INDUCER_TETR_ATC_Kd' , exp(13) , [exp(5) exp(15)] ...
activeNames(cell2mat(mte_phase2_params(:,1)),2) = mte_phase2_params(:,3);
activeNames(cell2mat(mte_phase2_params(:,1)),3) = mte_phase2_params(:,4);

%% training_full_params = ...
(...
11     , 'TXTL_PTET_sequestration_Kd' , exp(-0.5) , [exp(-2) exp(1)]
12     , 'TXTL_INDUCER_TETR_ATC_Kd' , exp(-2) , [exp(1) exp(5)]
13     , 'TXTL_INDUCER_LASR_AHL_Kd' , exp(13) , [exp(5) exp(15)] ...
);
activeNames(cell2mat(training_full_params(:,1)),2) = training_full_params(:,3);
activeNames(cell2mat(training_full_params(:,1)),3) = training_full_params(:,4);

training_full_params = ...
(...
1     , 'TX_elong_glob' , [exp(3.121) exp(1) exp(6)] %1 from est params above
2     , 'TL_elong_glob' , [exp(3.436) ,exp(1) exp(6)] %2 from est params above
);
activeNames(cell2mat(training_full_params(:,1)),2) = training_full_params(:,3);
activeNames(cell2mat(training_full_params(:,1)),3) = training_full_params(:,4);

estParamsIX = [7 21 23 28 31 33 37 39 40];
estParams = activeNames(estParamsIX,1)

estParams =
1x1 cell array
    ('TXTL_PTET_RNAPbound_Kd')
    ('TXTL_PLAC_RNAPbound_Kd')
    ('TXTL_RNAPbound_TERMINATION_RATE')
    ('TXTL_RIBOBOUND_TERMINATION_RATE')
    ('RNAP')
    ('Ribo')
    ('TXTL_PLAS_RNAPbound_Kd')
    ('TXTL_PLAS_TFBIND_Kd')
    ('TXTL_PLAS_TFRNAPbound_Kd')

f2 >> |

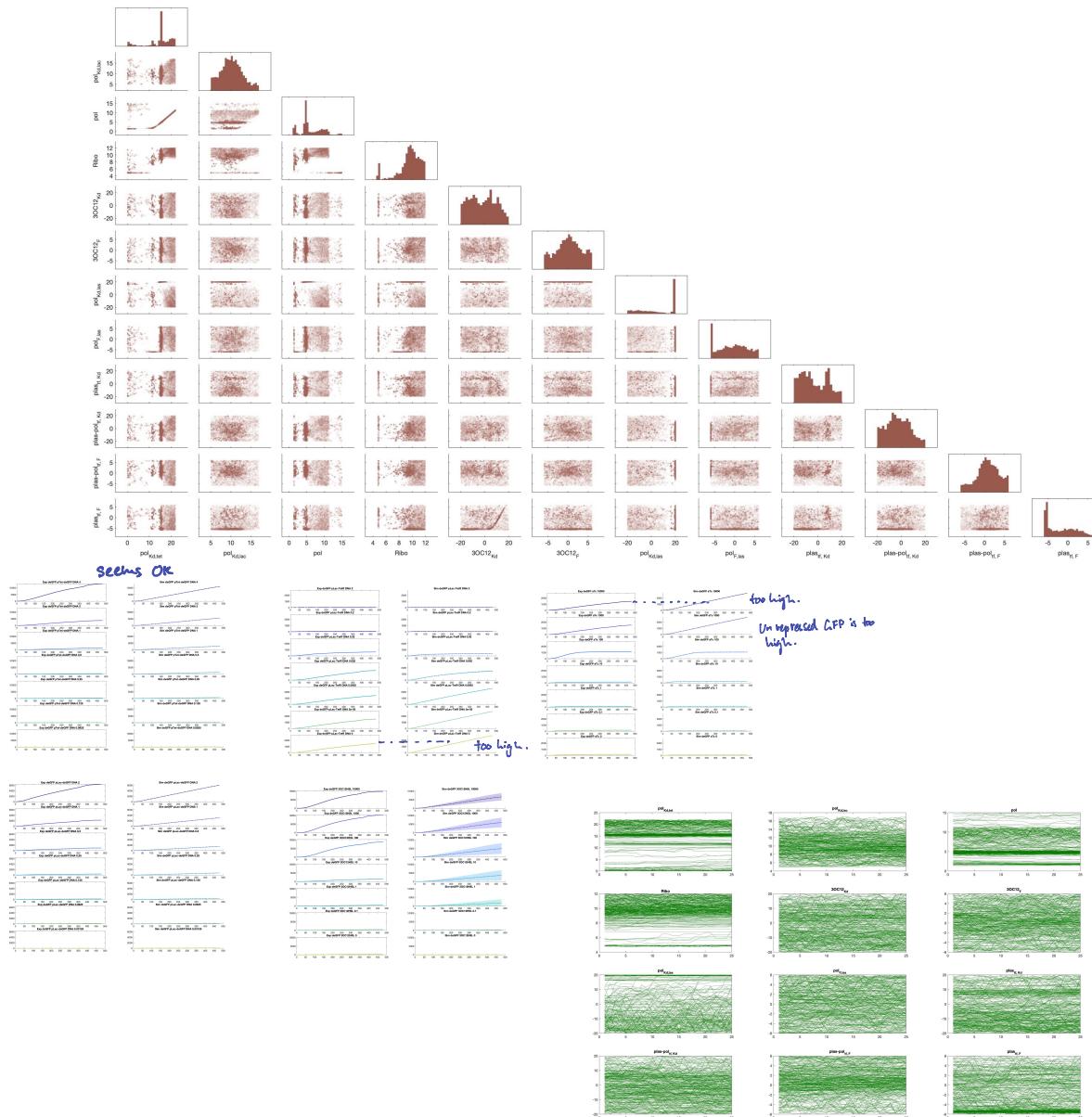
```

There are two DIFFERENT training full's:  
 training full -- pre May 6 commit  
 training full post may 6 commit

I guess after this i realized that i cannot just change the training full file, and started making A, B, C and so on.

Anyway, this is what the data looks like:

/Users/vipulsinghal/Dropbox/Documents/toolbox/txtlsm\_vsfork2017/  
 mcmc\_simbio/projects/proj\_ZSIFFL\_training/  
 simdata\_20190505\_023615\_1\_738/



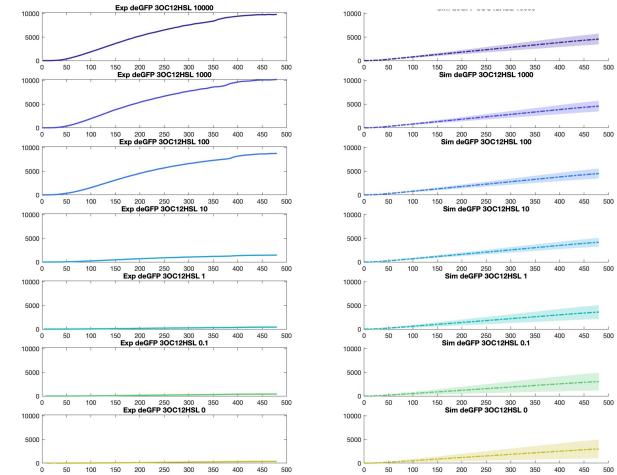
ZSIFFL\_training\_full -- AFTER the may 6 commit

```
estParamsIX = [7 21 23 28 31 33 35 37 39 48];
estParams = activebases(estParamsIX,1);
activebases(estParamsIX,1);

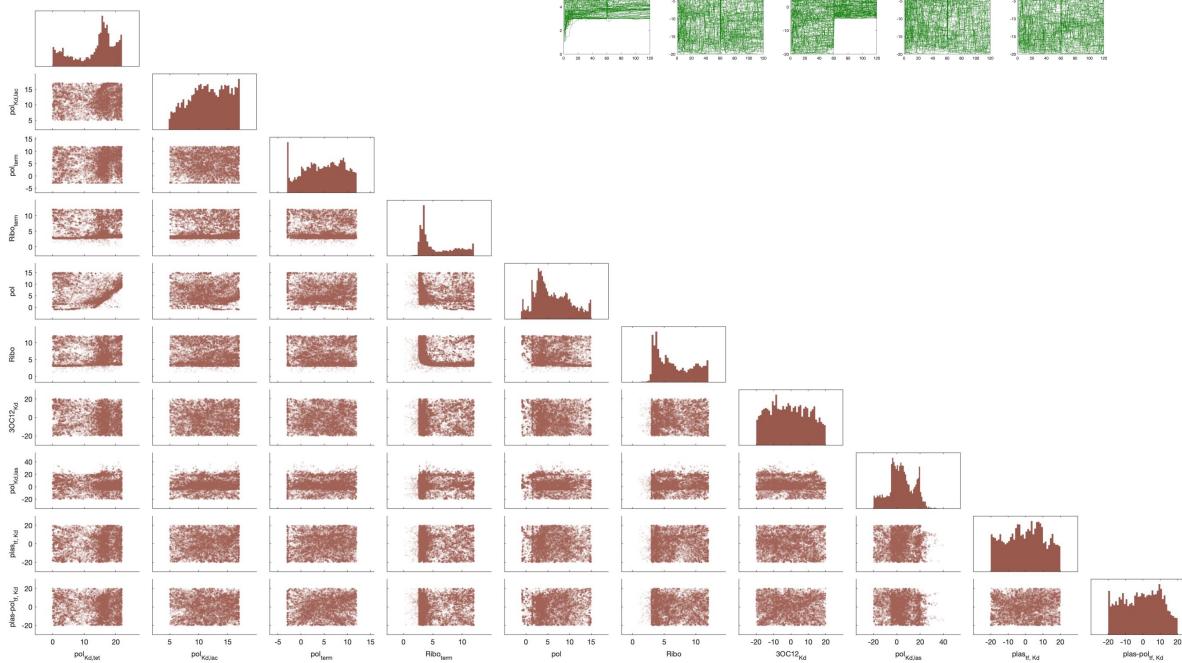
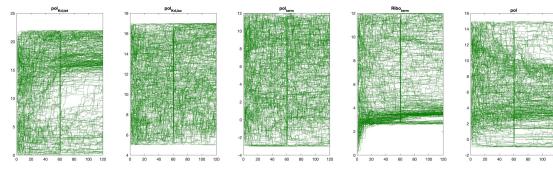
ans =
10x3 cell array

{'TXTL_PET_RNAbound_Kd'} {{1.5713e+07}} {1x2 double}
{'TXTL_PLAC_RNAbound_Kd'} {{3.6316e+04}} {1x2 double}
{'TXTL_RNABOUND_TERMINATION_RATE'} {{1.7639e+01}} {1x2 double}
{'TXTL_RNA80000_TERMINATION_RATE'} {{1.9593e+01}} {1x2 double}
{'RNAP'} {{3.0375e-02}} {1x2 double}
{'TXTL_INDUCER_LASR_AH_Kd'} {{365.8075}} {1x2 double}
{'TXTL_PLAC_RNAbound_Kd'} {{1.8686e+13}} {1x2 double}
{'TXTL_PLAS_TFBIND_Kd'} {{1.0135e-02}} {1x2 double}
{'TXTL_PLAS_TFRNAPbound_Kd'} {{7.3891}} {1x2 double}
```

/Users/vipulsinghal/Dropbox/  
Documents/toolbox/  
txtlsm\_vsfork2017/mcmc\_simbio/  
projects/proj\_ZSIFFL\_training/  
simdata\_20190507\_102955\_1\_1845/  
cornerplot20190507\_102955\_1\_1845  
Burned\_in.jpg



/Users/vipulsinghal/Dropbox/  
Documents/toolbox/  
txtlsm\_vsfork2017/mcmc\_simbio/  
projects/proj\_ZSIFFL\_training/  
simdata\_20190507\_102955\_1\_1845/  
trace20190507\_102955\_1\_1845Burn  
ed\_in.jpg



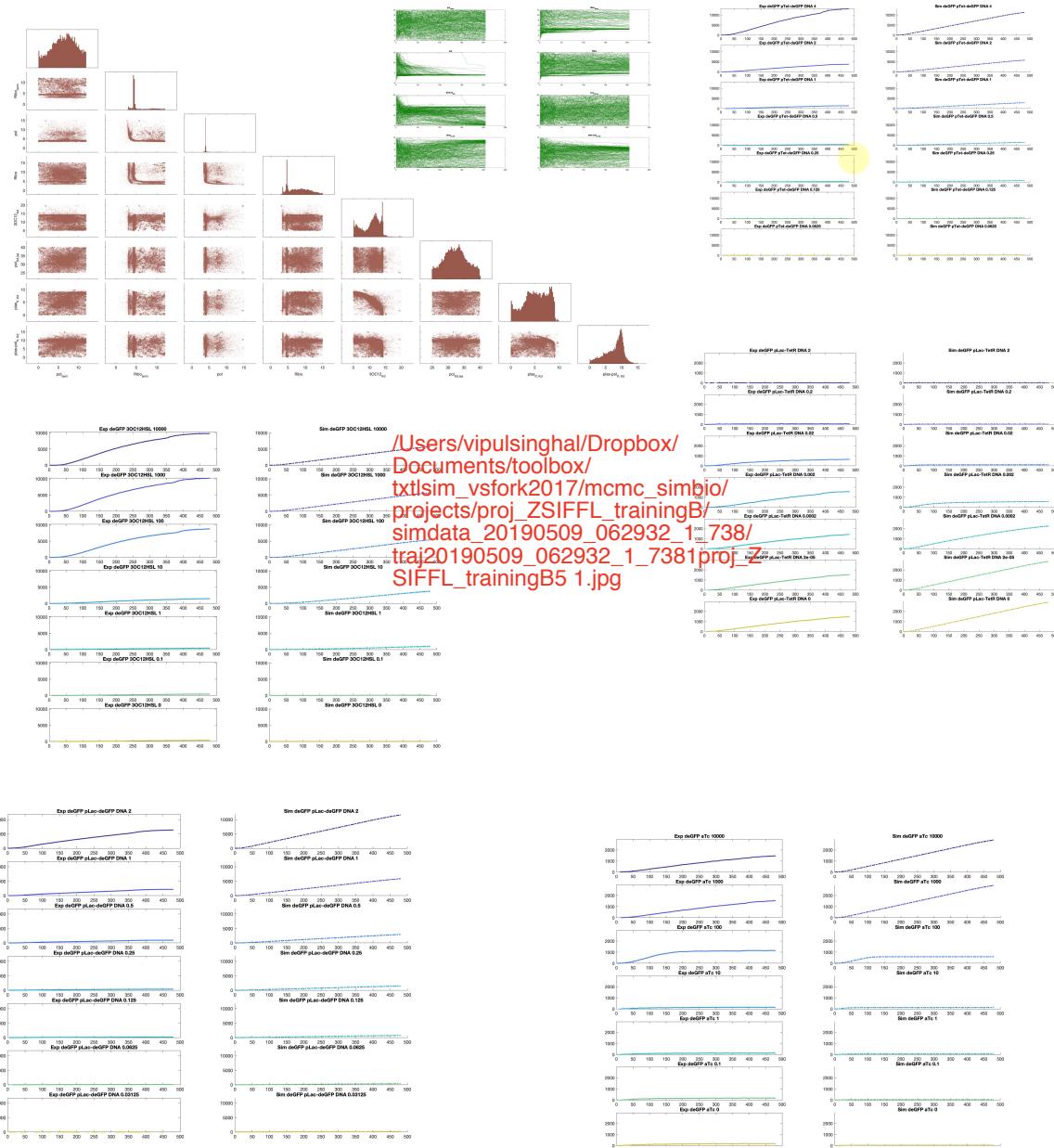
## ZSIFFL\_training\_fullB

here I thought that maybe the fact that the termination rates for the rnap and ribo were fixed was causing a bottleneck in the expression levels, limiting the simulated gfp from the plas-gfp to be much lower than the experimental data.

*Yup. I don't think the current list of params is the one I used for training-B5. it was*

long story short, In this sim, we estimate a larger set of params to try to get closer. And then in training C, that is where we really start to get close.

*only in training-B5  
that the termination  
rates were introduced.*



```

4 activeNames(cell2mat(mtet_phase1_params(:,1)),2) = mtet_phase1_params(:,3);
5 activeNames(cell2mat(mtet_phase1_params(:,1)),3) = mtet_phase1_params(:,4);
6
7 % The values estimated are:
8 mtet_phase2_params = ...
9 {...
10    1 , 'TX_elong_glob' , exp(2.3) , [exp(0) exp(5)]
11    2 , 'TL_elong_glob' , exp(3.7) , [exp(0) exp(6)]
12    3 , 'AGTPdeg_time' , exp(10.05) , [exp(8) exp(12)]
13    31 , 'RNAP' , exp(5.9) , [exp(1) exp(15)] %
14    32 , 'RNase' , exp(9.2) , [exp(7) exp(11)]
15    33 , 'Ribo' , exp(5.9) , [exp(1) exp(15)]
16    21 , 'TXTL_PLAC_RNAPbound_Kd' , exp(10.5) , [exp(5) exp(17)]
17    7 , 'TXTL_PTET_RNAPbound_Kd' , exp(17) , [exp(0) exp(22)]
18    11 , 'TXTL_PTET_sequestration_Kd' , exp(-2.7) , [exp(-10) exp(5)]
19    16 , 'TXTL_INDUCER_TETR_ATC_Kd' , exp(-6) , [exp(-15) exp(5)]...
20 };
21
22 activeNames(cell2mat(mtet_phase2_params(:,1)),2) = mtet_phase2_params(:,3);
23 activeNames(cell2mat(mtet_phase2_params(:,1)),3) = mtet_phase2_params(:,4);
24
25 % we also set the forward rate parameters, since those should not matter much, and any val
26 % the F rate parameters just set the timescale.
27
28 mtet_phase2_params = ...
29 {...
30    36 , 'TXTL_INDUCER_LASR_AHL_F' , exp(0) , [exp(-3) exp(5)]
31    38 , 'TXTL_PLAS_RNAPbound_F' , exp(0) , [exp(-3) exp(5)]
32    41 , 'TXTL_PLAS_TFRNAPbound_F' , exp(0) , [exp(-3) exp(5)]
33    42 , 'TXTL_PLAS_TFBIND_F' , exp(0) , [exp(-3) exp(5)] };
34
35 activeNames(cell2mat(mtet_phase2_params(:,1)),2) = mtet_phase2_params(:,3);
36 activeNames(cell2mat(mtet_phase2_params(:,1)),3) = mtet_phase2_params(:,4);
37
38
39 estParamsIX = [23 28 31 33 35 37 39 40];
40 estParams = activeNames(estParamsIX,1);

```

```

26 tsIDtouse = 1;
27 plotflag = true;
28 switch tsIDtouse
29 case 1 % this is after including the terminat
30   ts1 = '20190508_001705_1_1845';
31   ts2 = '20190508_213950_1_1107';
32   ts3 = '20190509_024244_1_738';
33   ts4 = '20190509_062932_1_738';
34   tstamp = {ts1 ts2 ts3 ts4};
35   nIterID = [1:7 1:9 1:6 1:2];
36   load([projdir '/simdata_' ts1 '/full_vari
37   'mi',...
38   'mcmc_info', 'data_info', 'ri'];
39 end
40 tsToSave = ts4;
41 mai.masterVector
42 marray_full = mcmc_get_walkers(tstamp,nIterID, pr
43 marray = marray_full(:,:,1:end);
44 clear marray_full
45 parnames = ...
46 {'pol_{term}'}
47 {'Ribo_{term}'}
48 {'pol'}
49 {'Ribo'}
50 {'30C12_{Kd}'}
51 {'pol_{Kd,las}'}
52 {'plas_{tf, Kd}'}
53 {'plas-pol_{tf, Kd}'};
54 % activeNames(estParamsIX,:);
55 %
56 % ans =
57 %

```

```

%<!--> EstimatedParams were precomputed, need to document this before a target.
EstimatedParams = [..];
%<!--> mcmc_info_ZSIFFL_training_fullC.m
mcmc_info_ZSIFFL_training_fullC

%<!--> ParamColumnToUse = 2;
paramVecToUse = EstimatedParams(:, ParamColumnToUse);
indicesMasterVectorEstimated = [1 3 5 21 23 15 30 31 32 2 6 28 33];
activNames = { .., param name, nominal value, range of parameters for uniform
'TX_elong_glob' , exp(2.6), [exp(0) exp(5)] ;
'TL_elong_glob' , exp(3.5), [exp(0) exp(6)] ;
'AGTPdeg_time' , exp(8.8), [exp(6) exp(11)] ;
'AGTPreg_ON' , exp(-3.9), [exp(-6) exp(-1)] ;
'AGTPdeg_rate' , exp(-9.9), [exp(-13) exp(-7)] ;
'TXTL_UTR1_Kd' , exp(1.7), [exp(0) exp(15)] ;
'TXTL_PTET_RNAPbound_Kd' , exp(14), [exp(0) exp(17)] ;
'TXTL_PTET_RNAPbound_F' , exp(1.5), [exp(0) exp(4)] ;
'TXTL_NTP_RNAP_1_Kd' , exp(2.9), [exp(0) exp(5)] ;
'TXTL_NTP_RNAP_2_Kd' , exp(14), [exp(10) exp(20)] ;
'TXTL_PTET_sequestration_Kd' , exp(12), [exp(3) exp(15)] ;
'TXTL_PTET_sequestration_F' , exp(1.5), [exp(-2) exp(5)] ;
'TL_AA_Kd' , exp(1.8), [exp(0) exp(10)] ;
'TL_AGP_Kd' , exp(11.5), [exp(10) exp(18)] ;
'TXTL_RNAdeg_Kd' , exp(15.2), [exp(7) exp(17)] ;
'TXTL_INDUCER_TETR_ATC_Kd' , exp(13), [exp(0) exp(18)] ;
'TXTL_INDUCER_TETR_ATC_F' , exp(2.6), [exp(-2) exp(5)] ;
'TXTL_DIMER_tet_Kd' , exp(13), [exp(7) exp(17)] ;
'TXTL_UTR1_F' , exp(2.6), [exp(-2) exp(5)] ;
'TXTL_UTR1_F' , exp(1.8), [exp(0) exp(12)] ;
'TXTL_PLAC_RNAPbound_Kd' , exp(13.8), [exp(5) exp(17)] ;
'TXTL_PLAC_RNAPbound_F' , exp(2.6), [exp(-2) exp(5)] ;
'TXTL_RNAPBOUND_TERMINATION_RATE' , exp(1.8), [exp(0) exp(12)] ;
'TXTL_NTP_RNAP_1_F' , exp(0), [exp(-2) exp(3)] ;
'TXTL_NTP_RNAP_2_F' , exp(0), [exp(-2) exp(3)] ;
'TL_AGP_F' , exp(-1.2), [exp(-4) exp(3)] ;
'TXTL_RIBOROUND_TERMINATION_RATE' , exp(2.3), [exp(0) exp(12)] ;
'TXTL_RNAdeg_F' , exp(0), [exp(-3) exp(3)] ;
'TXTL_RNAdeg_Kc' , exp(-0.45), [exp(-5) exp(3)] ;
'RNP' , exp(1.449), [exp(-1) exp(8)] ;
'RNase' , exp(8.5), [exp(5) exp(18)] ;
'RNA' , exp(3.67), [exp(0) exp(6)] ;
'TXTL_PROT_deGFP_MATURATION' , exp(-6.07), [exp(-9) exp(-3)] ;
'TXTL_INDUCER_LASR_AHL_Kd' , exp(-2), [exp(5) exp(20)] %36-1 ;
'TXTL_INDUCER_LASR_AHL_F' , exp(0), [exp(-6) exp(6)] %37-1 ;
'TXTL_PLAS_RNAPbound_Kd' , exp(30), [exp(25) exp(40)] %38-1 ;
'TXTL_PLAS_RNAPbound_F' , exp(3), [exp(-6) exp(6)] %39-1 pol ;
'TXTL_PLAS_TFBIND_Kd' , exp(0), [exp(0) exp(10)] %40-1 pol ;
'TXTL_PLAS_TFBIND_F' , exp(0), [exp(-6) exp(6)] %41-1 pol ;
'TXTL_PLAS_TFBIND_F' , exp(0), [exp(-6) exp(6)] %42-1 pol ;
% Set the master vector values that are set from the values estimated in "vnpr_F"
% Set the master vector values that were already fixed in "vnpr_F"
prefixedParams = { ...
4 'AGTPreg_ON' , exp( -3.9120)
34 'TXTL_PROT_deGFP_MATURATION' , exp( -6.0748)
8 'TXTL_PTET_RNAPbound_F' , exp( 1.5000)
9 'TXTL_NTP_RNAP_1_Kd' , exp( 2.9459)
10 'TXTL_NTP_RNAP_2_Kd' , exp( 13.9970)
13 'TL_AA_Kd' , exp( 6.5566)
14 'TL_AGP_Kd' , exp( 14.5090)
20 'TXTL_UTR1_F' , exp( -0.2000)
22 'TXTL_PLAC_RNAPbound_F' , exp( 1.5000)
24 'TXTL_NTP_RNAP_1_F' , exp( 0)
25 'TXTL_NTP_RNAP_2_F' , exp( 0)
26 'TL_AA_F' , exp( -0.3000)
27 'TL_AGP_F' , exp( -1.2000)
29 'TXTL_RNAdeg_F' , exp( 0)); % checked a

% set the prefixed params elements in master vector to the values in

mtet_phase1_params = ...
{...
7 , 'TXTL_PTET_RNAPbound_Kd' , exp(14) , [exp(0) exp(17)] ;
11 , 'TXTL_PTET_sequestration_Kd' , exp(-1) , [exp(-10) exp(5)] ;
12 , 'TXTL_PTET_sequestration_F' , exp(1.214) , [exp(-2) exp(5)] ;
16 , 'TXTL_INDUCER_TETR_ATC_Kd' , exp(-2) , [exp(-15) exp(5)] ;
17 , 'TXTL_INDUCER_TETR_ATC_F' , exp(1.577) , [exp(-2) exp(5)] ;
18 , 'TXTL_DIMER_tet_Kd' , exp(-10) , [exp(-20) exp(-7)] ;
19 , 'TXTL_DIMER_tet_F' , exp(14.447) , [exp(-2) exp(5)] ;
};

activNames(cell2mat(mtet_phase1_params(:,1)),2) = mtet_phase1_params(:,2);
activNames(cell2mat(mtet_phase1_params(:,1)),3) = mtet_phase1_params(:,3);

% next we set the parameters estimated from mcmc_info_ZSIFFL_mtet_phase2.m

% The values estimated are:
mtet_phase2_params = ...
{...
1 , 'TX_elong_glob' , exp(2.3) , [exp(0) exp(7)] ; %1 from est
2 , 'TL_elong_glob' , exp(3.7) , [exp(0) exp(7)] ; %2 from est
3 , 'AGTPdeg_time' , exp(18.05) , [exp(8) exp(12)] ; %3 from est
31 , 'RNAP' , exp(5.9) , [exp(1) exp(15)] ; %31 31% from est
32 , 'RNP' , exp(1.7) , [exp(1) exp(15)] ; %32 from est
33 , 'Riboz' , exp(5.9) , [exp(1) exp(15)] ; %33 from est
21 , 'TXTL_PLAC_RNAPbound_Kd' , exp(18.5) , [exp(5) exp(25)] ; %21 from est
7 , 'TXTL_PTET_RNAPbound_Kd' , exp(17) , [exp(5) exp(25)] ;
11 , 'TXTL_PTET_sequestration_Kd' , exp(-2.7) , [exp(-10) exp(10)] ;
16 , 'TXTL_INDUCER_TETR_ATC_Kd' , exp(-6) , [exp(-15) exp(15)] ;
};

activNames(cell2mat(mtet_phase2_params(:,1)),2) = mtet_phase2_params(:,2);
activNames(cell2mat(mtet_phase2_params(:,1)),3) = mtet_phase2_params(:,3);

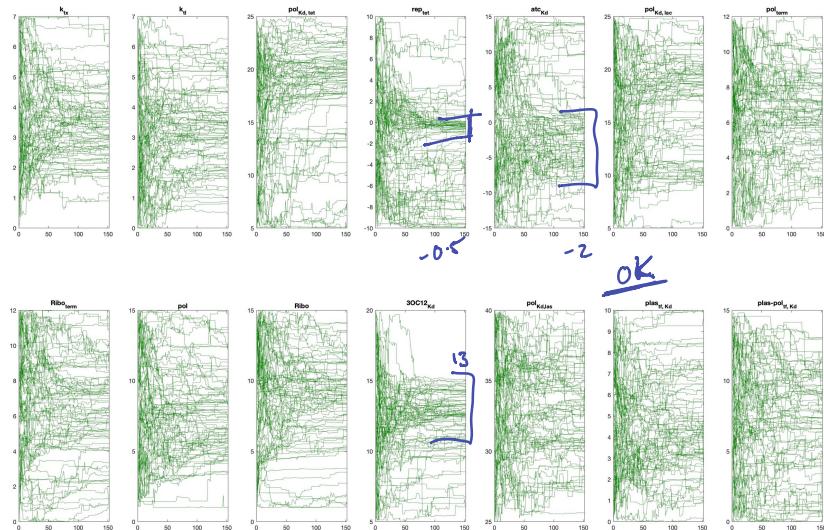
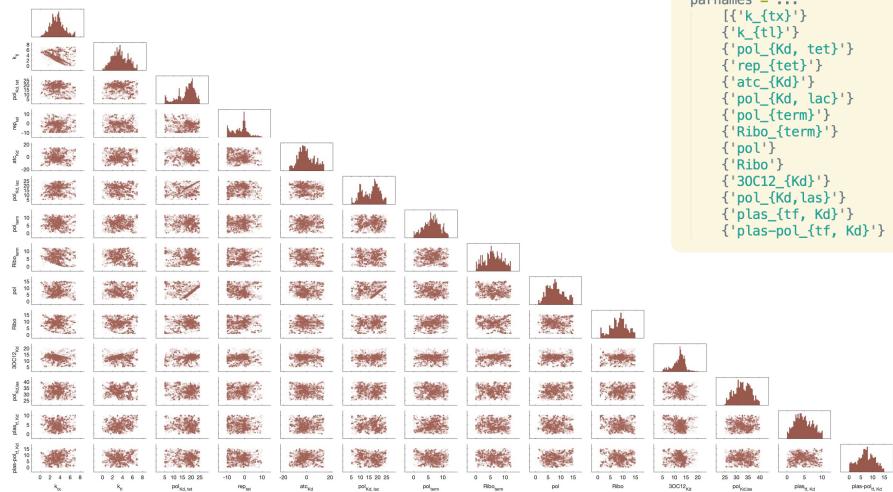
estParamsIX = [1 2 7 11 16 21 23 28 31 33 35 37 39 40];
estParams = activeNames(estParamsIX,1);

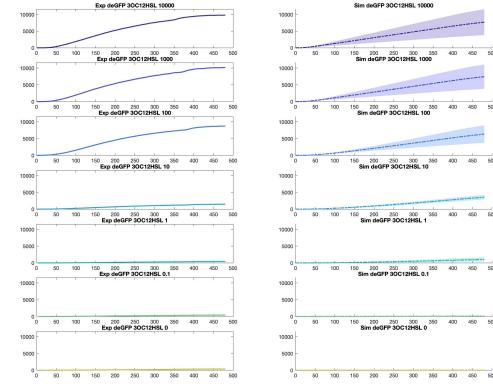
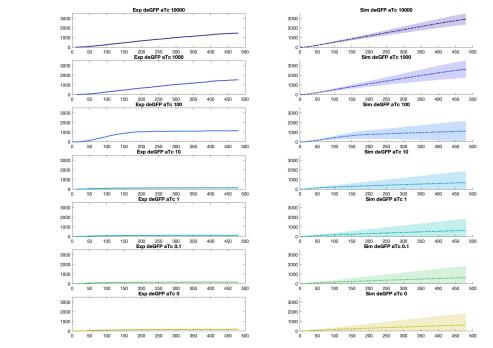
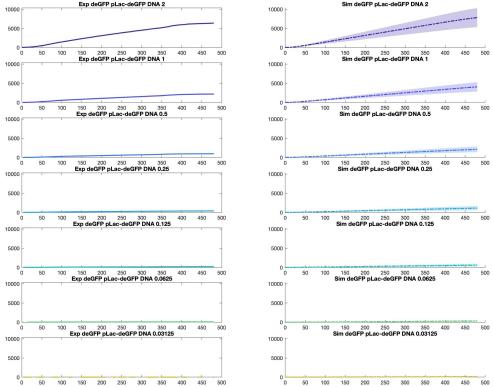
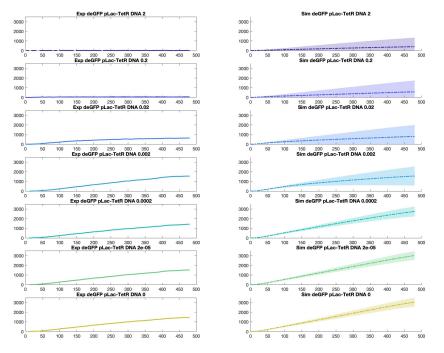
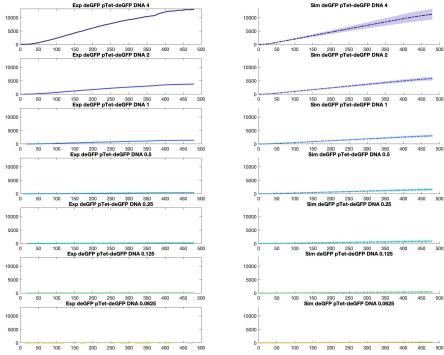
```

```

plotflag = true;
switch tsIDtouse
case 1 % this is after including the termination parameter
    ts1 = '20190509_092707_1_1476';
    ts2 = '20190509_160552_1_1476';
    ts3 = '20190509_160552_2_738';
    ts4 = '20190509_160552_3_554';
    ts5 = '20190510_064333_1_369';
    ts6 = '20190510_064333_2_185';
    ts7 = '20190510_064333_3_74';
    ts8 = '20190511_014023_1_74';
    tstamp = [ts1 ts2 ts3 ts4 ts5 ts6 ts7 ts8];
    nIterID = [1:1:1:20 1:20 1:20 1:20 1:8 1:5];
    load([projdir '/simdata_' ts1 '/full_variable_set.mat']);
    'mcmc_info', 'data_info', 'ri');
end
tsToSave = ts8;
mai.masterVector;
marray_full = mcmc_get_walkers(tstamp,nIterID, projdir);
marray = marray_full(:, :, 1:end);
clear marray_full
parnames = ...
{ {'K_{tx}'}
{ 'K_{tl}'}
{ 'pol_{Kd, tet}'}
{ 'rep_{tet}'}
{ 'atc_{Kd}'}
{ 'pol_{Kd, lac}'}
{ 'pol_{term}'}
{ 'Ribo_{term}'}
{ 'pol' }
{ 'Ribo' }
{ '3OC12_{Kd}' }
{ 'pol_{Kd, las}' }
{ 'plas_{tf, Kd}' }
{ 'plas-pol_{tf, Kd}' } };

```

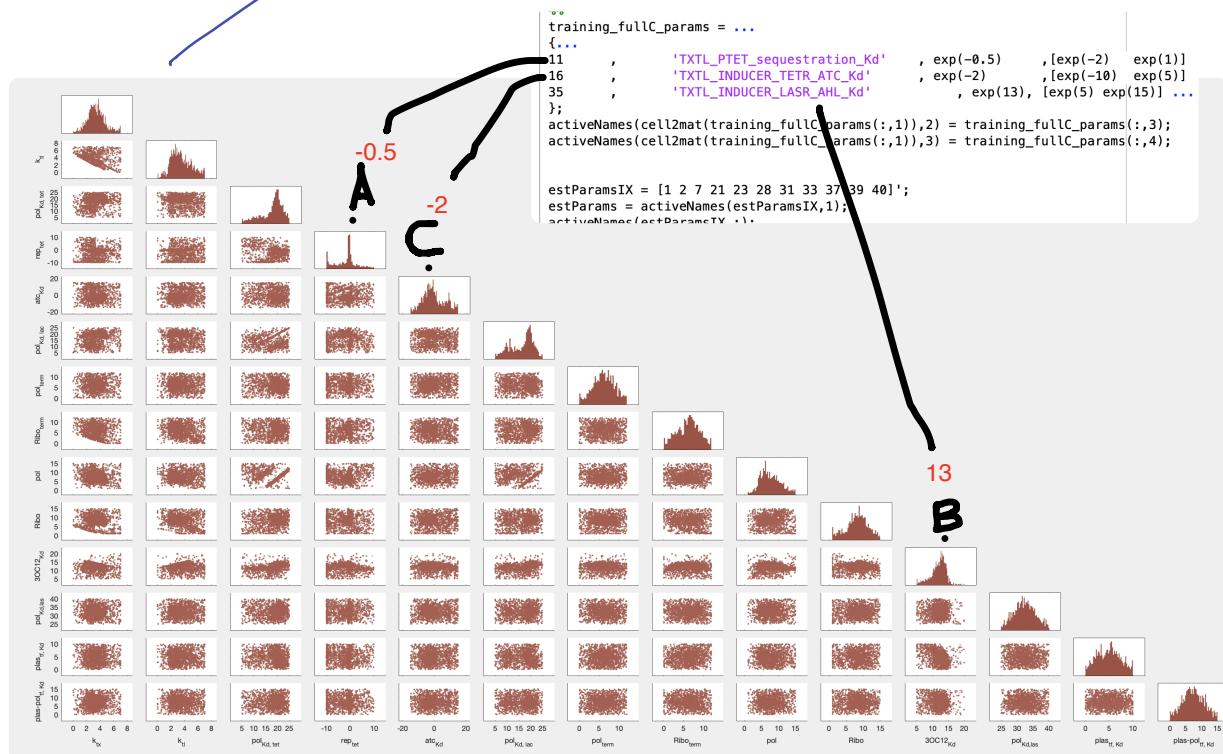




going to do the restriction procedure thing to slice out parameters, and then fix them in a consistent way. you cannot just pick parameters by looking at the plot below. if you fix parameters A and B, you have to make sure they are consistent, in the sense that there are points in the distribution that have that combination of A and B. This can be done sequentially:

see below.

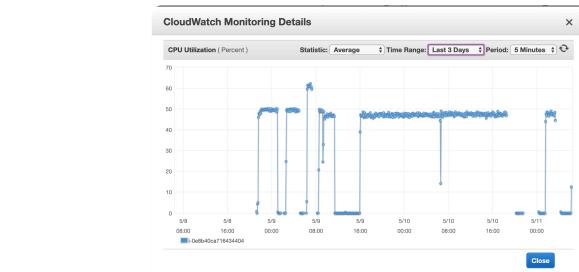
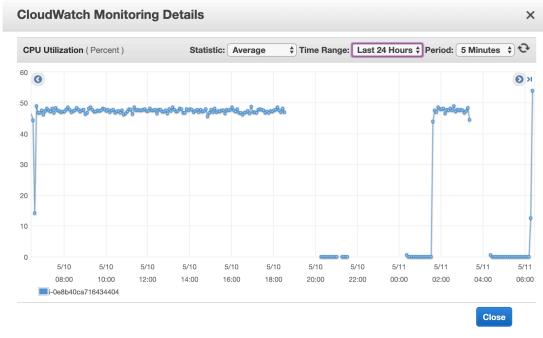
commit: [f5a61358cd9c1f4f24b5d6bd140bbce5d5f0719e](#)



```

573 %
574 % 20190511_062400_1_738
575 pro=MFFL_TrainingD('stepSize', 1.3, ...
576 'nWt', 40, ...
577 'nPoin', 50*400, ...
578 'thining', 10, ...
579 'niter', 20, ...
580 'parallel', true, ...
581 'poolsize', 48, ...
582 'temperatureLadder', [0.0001 0.00005 0.00001], ...
583 'stepLadder', [1])% CURRENT
584 %
585 %
586 %
587 %
588 %

```

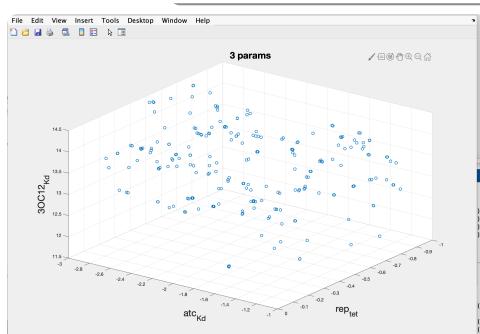


```

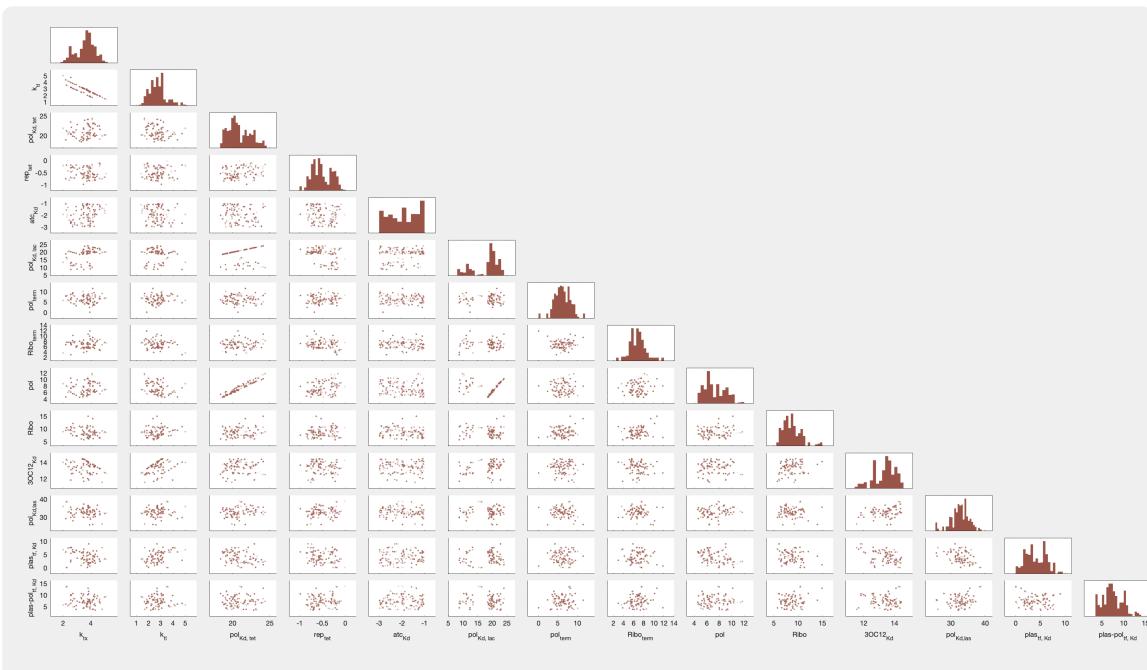
parIDs = [4 5 11];
% parRanges(parIDs, :) = [-1 0 ;
%   1 8;
%   11 15];
parRanges(parIDs, :) = [-1 0 ;
%   1 8;
%   11 14.5];
array_cut = ncnc_cut(array(:, 1:end,(end - 40):end), parIDs, flipud(parRanges(parIDs, :))');
mcut = array_cut(parIDs, :,1);
mcnc_3D(mcut(1,:)', parnames(parIDs), '3 params');

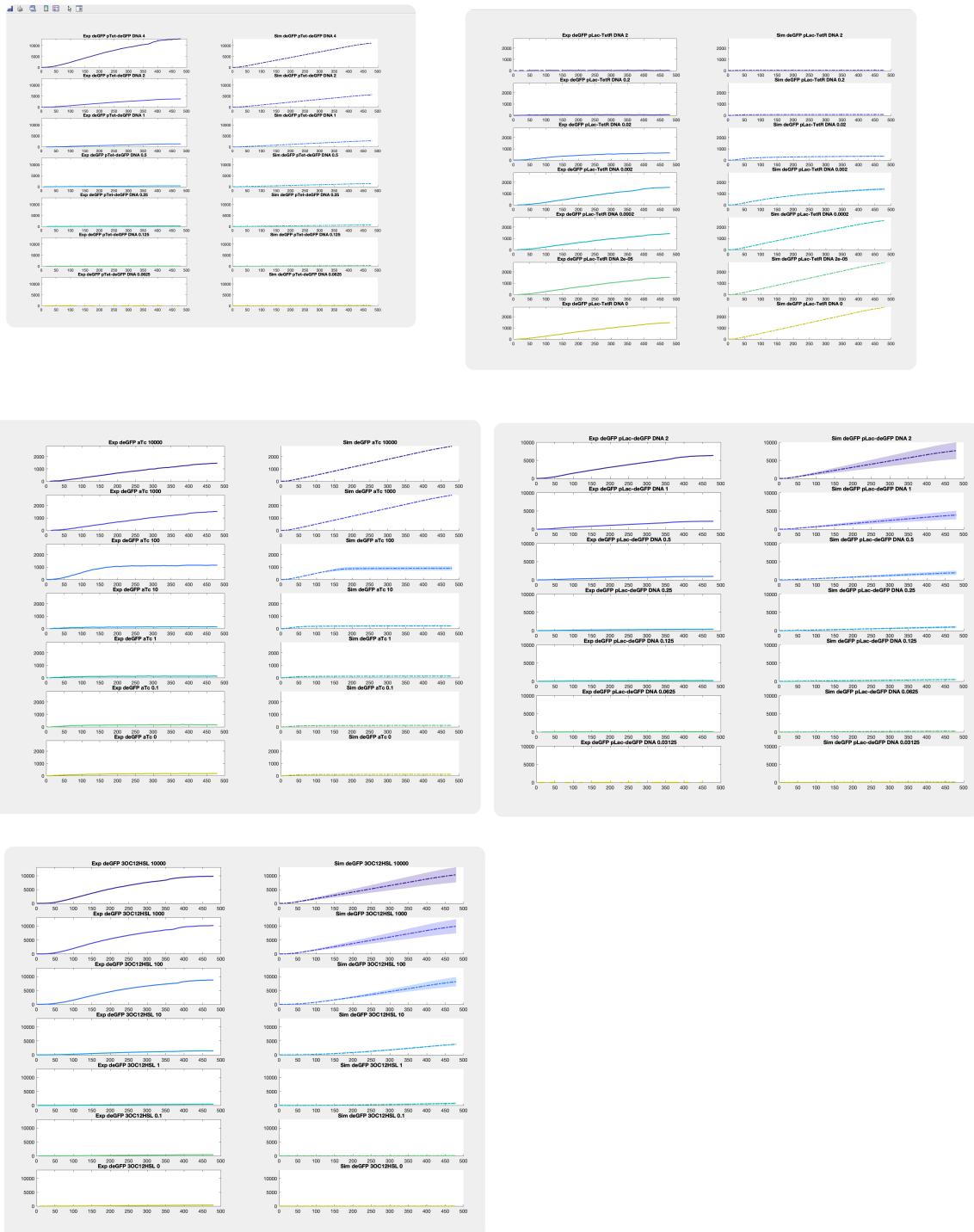
mcnc_plot(array_cut, parnames());
%save matfig, figsize, 'savejpeg', false, ...
%prodif, prodif, 'temp', t3t0ave, 'signamenamestring', 'BurnedIn';
mcnc_3D(mcut(1,:)', parnames(parIDs), '3 params')

```

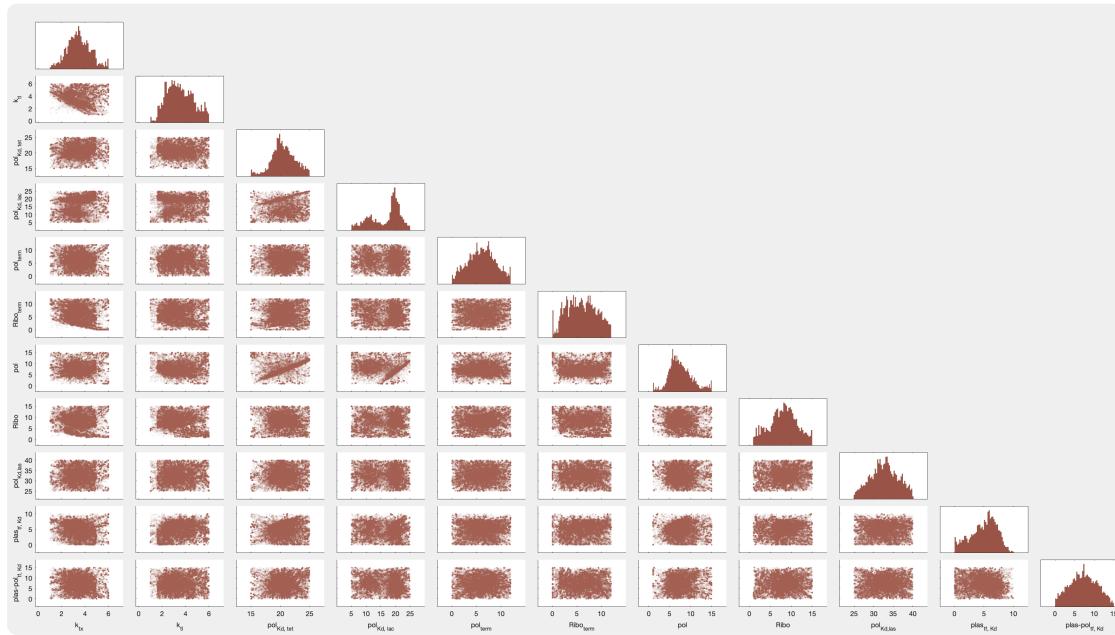


analysis  
training fullC  
(fixing /  
restricting)



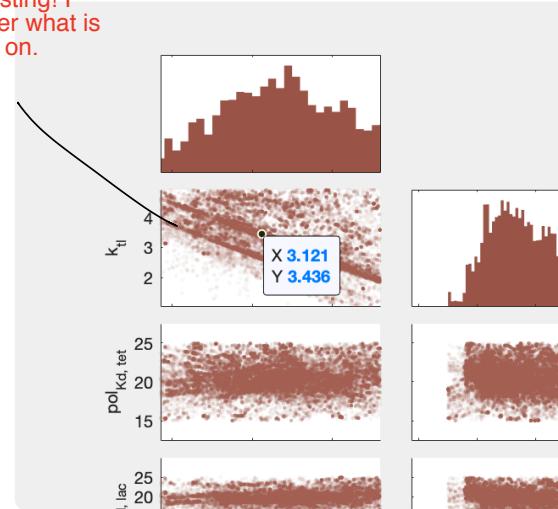
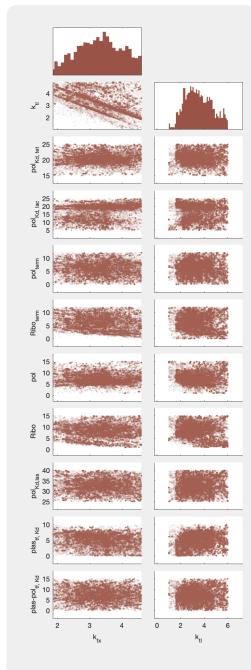


in fullID, I have the following. I think I am going to fix the kTX and kTL and estimate the rest. there are potentially 2 non identifiability trios: ktx, pol and polterm as 1, and ktl, ribo, riboterm as the second. Maybe the problem gets easier if I fix either pol or ktx (dont want to fix the terms I think) Actually, I want to do 3 sims, with each of these fixed, and see what happens.



lets fix ktx and ktl first:

why are there two  
lines! so  
interesting! I  
wonder what is  
going on.



this spotty ness you see  
is the chains getting  
stuck, because the  
temperature is too low.  
need acceptance of  
0.23, and see the temp  
in training E below, that  
gets a good mixing, and  
is not spotty.

talk about this  
spottiness in the supp  
info.

fix to these values. start training\_fullE

Trainning FullE -- 84% rejection with super high temp of 1.5k (.02% of signal) Seems like the temp should be slightly higher than even this. but its ok, i will stay at this for now. 40 iters == 14 hours. started at like 11.

```
proj_ZSIFFL_trainingE('stepSize', 1.2,...  
'nW', 480,...  
'nPPoints', 50*480,...  
'thinning', 10,...  
'nIter', 40,...  
'parallel', true, ...  
'poolsize', 48,...  
'temperatureLadder', [ 0.0002],...  
'stepLadder', [1])
```

```
GMCMC: 84.0% [*****] 00:00:01  
83% rejected  
GMCMC: 83.0% [*****] 00:00:01  
82% rejected  
GMCMC: 82.0% [*****] 00:00:01  
81% rejected  
GMCMC: 81.0% [*****] 00:00:01  
80% rejected  
GMCMC: 80.0% [*****] 00:00:01  
79% rejected  
GMCMC: 79.0% [*****] 00:00:01  
78% rejected  
GMCMC: 78.0% [*****] 00:00:01  
77% rejected  
GMCMC: 77.0% [*****] 00:00:01  
76% rejected  
GMCMC: 76.0% [*****] 00:00:01  
75% rejected  
GMCMC: 75.0% [*****] 00:00:01  
74% rejected  
GMCMC: 74.0% [*****] 00:00:01  
73% rejected  
GMCMC: 73.0% [*****] 00:00:01  
72% rejected  
GMCMC: 72.0% [*****] 00:00:01  
71% rejected  
GMCMC: 71.0% [*****] 00:00:01  
70% rejected  
GMCMC: 70.0% [*****] 00:00:01  
69% rejected  
GMCMC: 69.0% [*****] 00:00:01  
68% rejected  
GMCMC: 68.0% [*****] 00:00:01  
67% rejected  
GMCMC: 67.0% [*****] 00:00:01  
66% rejected  
GMCMC: 66.0% [*****] 00:00:01  
65% rejected  
GMCMC: 65.0% [*****] 00:00:01  
64% rejected  
GMCMC: 64.0% [*****] 00:00:01  
63% rejected  
GMCMC: 63.0% [*****] 00:00:01  
62% rejected  
GMCMC: 62.0% [*****] 00:00:01  
61% rejected  
GMCMC: 61.0% [*****] 00:00:01  
60% rejected  
GMCMC: 60.0% [*****] 00:00:01  
59% rejected  
GMCMC: 58.0% [*****] 00:00:01  
57% rejected  
GMCMC: 56.0% [*****] 00:00:01  
55% rejected  
GMCMC: 54.0% [*****] 00:00:01  
53% rejected  
GMCMC: 52.0% [*****] 00:00:01  
51% rejected  
GMCMC: 50.0% [*****] 00:00:01  
49% rejected  
GMCMC: 48.0% [*****] 00:00:01  
47% rejected  
GMCMC: 45.0% [*****] 00:00:01  
44% rejected  
GMCMC: 42.0% [*****] 00:00:01  
41% rejected  
GMCMC: 39.0% [*****] 00:00:01  
38% rejected  
GMCMC: 36.0% [*****] 00:00:01  
35% rejected  
GMCMC: 33.0% [*****] 00:00:01  
32% rejected  
GMCMC: 30.0% [*****] 00:00:01  
29% rejected  
GMCMC: 28.0% [*****] 00:00:01  
27% rejected  
GMCMC: 26.0% [*****] 00:00:01  
25% rejected  
GMCMC: 24.0% [*****] 00:00:01  
23% rejected  
GMCMC: 22.0% [*****] 00:00:01  
21% rejected  
GMCMC: 20.0% [*****] 00:00:01  
19% rejected  
GMCMC: 18.0% [*****] 00:00:01  
17% rejected  
GMCMC: 16.0% [*****] 00:00:01  
15% rejected  
GMCMC: 14.0% [*****] 00:00:01  
13% rejected  
GMCMC: 12.0% [*****] 00:00:01  
11% rejected  
GMCMC: 10.0% [*****] 00:00:01  
9% rejected  
GMCMC: 8.0% [*****] 00:00:01  
7% rejected  
GMCMC: 6.0% [*****] 00:00:01  
5% rejected  
GMCMC: 4.0% [*****] 00:00:01  
3% rejected  
GMCMC: 2.0% [*****] 00:00:01  
1% rejected  
GMCMC: 0.0% [*****] 00:00:01  
0% rejected  
Elapsed time is 1356.065360 seconds.  
Iteration number 4.  
starting mcmc 4  
current step size: 1.200000e+00
```

```
GMCMC: 18.3% [*****] 00:00:23  
81% rejected  
GMCMC: 17.3% [*****] 00:00:23  
80% rejected  
GMCMC: 16.3% [*****] 00:00:23  
79% rejected  
GMCMC: 15.3% [*****] 00:00:23  
78% rejected  
GMCMC: 14.3% [*****] 00:00:23  
77% rejected  
GMCMC: 13.3% [*****] 00:00:23  
76% rejected  
GMCMC: 12.3% [*****] 00:00:23  
75% rejected  
GMCMC: 11.3% [*****] 00:00:23  
74% rejected  
GMCMC: 10.3% [*****] 00:00:23  
73% rejected  
GMCMC: 9.3% [*****] 00:00:23  
72% rejected  
GMCMC: 8.3% [*****] 00:00:23  
71% rejected  
GMCMC: 7.3% [*****] 00:00:23  
70% rejected  
GMCMC: 6.3% [*****] 00:00:23  
69% rejected  
GMCMC: 5.3% [*****] 00:00:23  
68% rejected  
GMCMC: 4.3% [*****] 00:00:23  
67% rejected  
GMCMC: 3.3% [*****] 00:00:23  
66% rejected  
GMCMC: 2.3% [*****] 00:00:23  
65% rejected  
GMCMC: 1.3% [*****] 00:00:23  
64% rejected  
GMCMC: 0.3% [*****] 00:00:23  
63% rejected  
GMCMC: 0.0% [*****] 00:00:23  
62% rejected  
Elapsed time is 1356.065360 seconds.  
Iteration number 4.  
starting mcmc 4  
current step size: 1.200000e+00
```

posterior distributions are not spotty, ie, the rejection probability is not too high. ie the chains are not getting stuck. i need rejection to be around 77%. this is still too high. going to raise temperature more, or lower step size.



```
% plot data from existing simulations.  
tsIDtouse = 1;  
plotflag = true;  
switch tsIDtouse  
    case 1 % this is after including the termination parameters.  
        ts1 = '20190512_033128_1_1476';  
        ts2 = '20190512_864547_1_1476';  
        tstamp = (ts1 ts2);  
        nIterID = {1:1:6};  
        load(projdir '/simdata_'.ts1 '/full_variable_set'.ts1 '.mat');  
        nmc_info  
    end  
    tsIDtouse = 2; % (end)  
    nmc_info  
    nmc_full = nmc_get_walkers(tstamp,nIterID,projdir);  
    marray = marray_full(:,1:1);  
    clear marray_full  
    parnames = {...  
        '(pol_1,term)'  
        '(pol_1d,term)'  
        '(pol_1,term)'  
        '(Ribo,term)'  
        '(pol)'  
        '(pol_1d,term)'  
        '(plas,(tf,Kd))'  
        '(plas-pol_(tf,Kd))' };
```

/Users/vipulsinghal/Dropbox/Documents/toolbox/txtlsim\_vsfork2017/mcmc\_simbio/projects/analysis\_ZSIFFL\_training\_fullE.m

why are there 2 lines here, what is going on? so intreseting. can try to plot 3 at a time 3d Plots to try to see if you can see a trend for why there are 2 seaprate lines.

also, what is going on with this knee behavior?

These sims need to run to exhaustion / till its is super clean. Then these trends will be super clear.

ONCE THIS PAPER IS DONE, EMAIL RMM ABOUT APPLYING FOR AWS GRANTS. TELL HIM HOW MUCH I HAVE SPENT!

Can also look at applying for other grants.

Search by keyword

Type	Instance type	State	Capacity
	m5.12xlarge	<span>🟡 open</span>	-
	c5.9xlarge	<span>🔴 cancelled</span>	-
	c4.8xlarge	<span>🔴 cancelled</span>	i-0adb83ee8de36...

