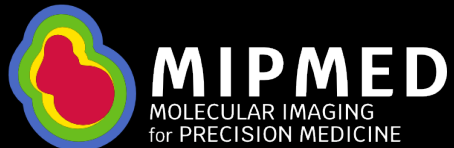


✉ [dgomez@ibecbarcelona.eu](mailto:dgomez@ibecbarcelona.eu)

# Fira Fair Data 2024

**David Gomez-Cabeza**  
Postdoctoral Researcher



# *My Datasets*

Computational  
Simulations and  
Scripts

Microscopy  
Images

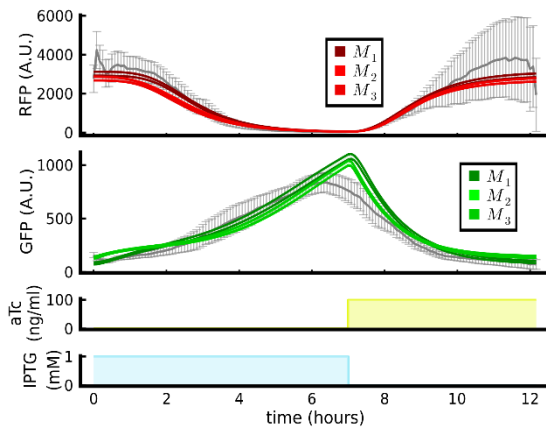
Nuclear Magnetic  
Resonance Spectra

Magnetic Resonance  
Images (MRI)



# My Datasets

## Computational Simulations and Scripts



## Microscopy Images

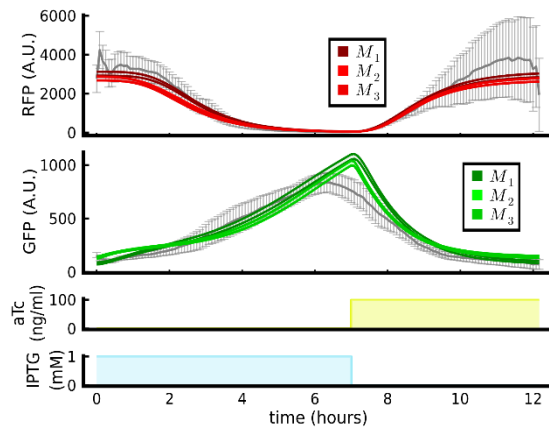
## Nuclear Magnetic Resonance Spectra

## Magnetic Resonance Images (MRI)

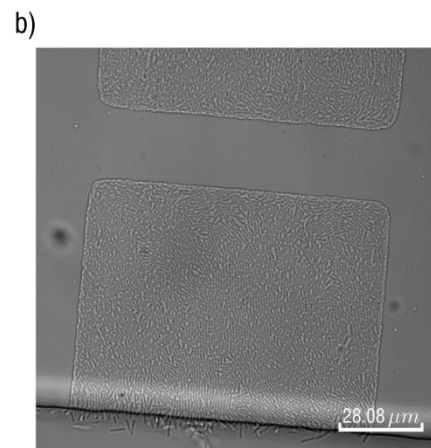
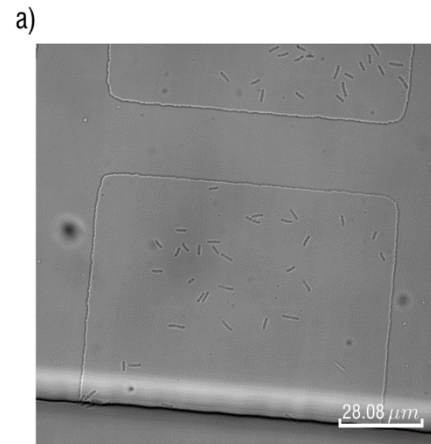
```
1 Function reconstructData(paths)
2
3 ##### OBSERVABLES #####
4
5 m = length(paths);
6
7 DataAll = Array{Any,1}(undef, m)
8
9 for i in 1:m
10     DataAll[i] = Matrix(CSV.read(paths[i], DataFrame));
11 end
12 stslm = maximum([size(DataAll[i],1) for i in 1:m]);
13 stsl = reshape([size(DataAll[i],1) for i in 1:m], 1, m);
14
15 obser = 2;
16 obSta = Array{Int,2}(undef, 1, 2)
17 obSta[1,:] = [1,2];
18
19 Means = Array{Float64,3}(undef, stslm, m, obser);
20 Error = Array{Float64,3}(undef, stslm, m, obser);
21 stl = Array{Int,2}(undef, stslm, m)*0
22 stl2 = Array{Int,2}(undef, stslm, m)
23
24 YObs = Array{Float64,2}(undef, 3, m);
25 tml = maximum([length(DataAll[i],1):DataAll[i][end,1] for i in 1:m]);
26 ts = Array{Float64,2}(undef, tml, m);
27 tlp = Array{Float64,1}(undef, m);
28
29 ms = collect(2:2:obser*2);
30 for i in 1:m
31     stl[3:length(DataAll[i]),1] = convert{Int, DataAll[i][1:end,1]};
32     stl[1:length(DataAll[i]),1] = convert{Int, DataAll[i][1:end,1]};
33     ts[1:length(DataAll[i]),1] = DataAll[i][end,1];
34     ts[1,i] = 1e-20;
35     for j in 1:obser
```

# My Datasets

## Computational Simulations and Scripts



## Microscopy Images



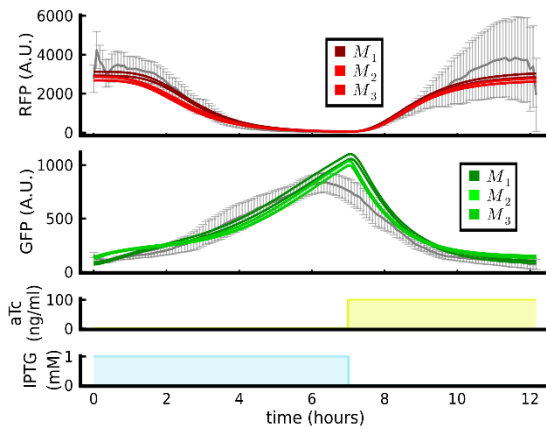
## Nuclear Magnetic Resonance Spectra

## Magnetic Resonance Images (MRI)

```
Function_restructDatInf(paths)
1
2
3 ##### OBSERVABLES #####
4
5 m = length(paths);
6
7 DataAll = Array{Any,1}(undef, m)
8
9 for i in 1:m
10 DataAll[i] = Matrix(CSV_read(paths[i], DataFrame));
11 end
12 stslm = maximum([size(DataAll[i]) for i in 1:m]);
13 stsl = reshape([size(DataAll[i]) for i in 1:m], 1, m);
14
15 obser = 2;
16 obSta = Array{Int,2}(undef, 1, 2)
17 obSta[1,:] = [1,2];
18
19 Means = Array{Float64,3}(undef, stslm, m, obser);
20 Errors = Array{Float64,3}(undef, stslm, m, obser);
21 stS = Array{Int,2}(undef, stslm, m)*0
22 stS2 = Array{Int,2}(undef, stslm, m)
23
24 YObs = Array{Float64,2}(undef, 3, m);
25 tml = maximum([length(DataAll[i][1,1]:DataAll[i][1,end,1]) for i in 1:m]);
26 ts = Array{Float64,2}(undef, tml, m);
27 tlp = Array{Float64,1}(undef, m);
28
29 ms = collect(2:2:obser*2);
30 for i in 1:m
31 stS[3:length(DataAll[i][1,1]:DataAll[i][1,end,1])] = convert{Int, DataAll[i][1,end,1]};
32 stS2[3:length(DataAll[i][1,1]:DataAll[i][1,end,1])] = convert{Int, DataAll[i][1,end,1]};
33 ts[1:length(DataAll[i][1,1]:DataAll[i][1,end,1])] = convert{Int, DataAll[i][1,1]};
34 ts[3,1] = 1e-20;
35 for j in 1:obser
```

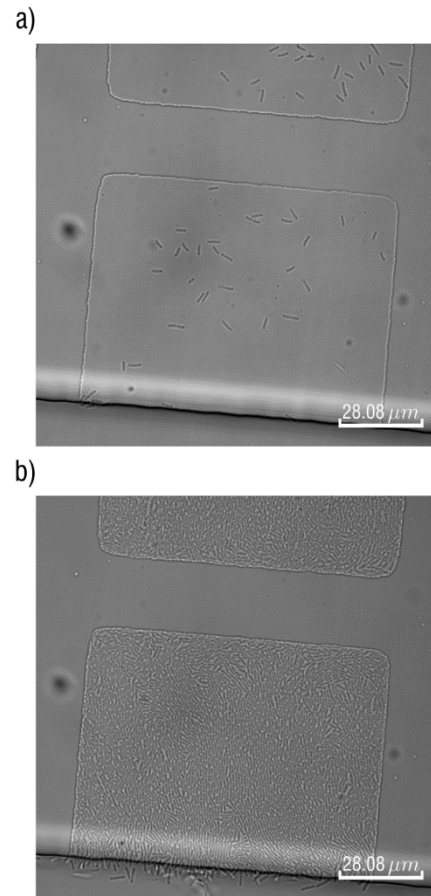
# My Datasets

## Computational Simulations and Scripts

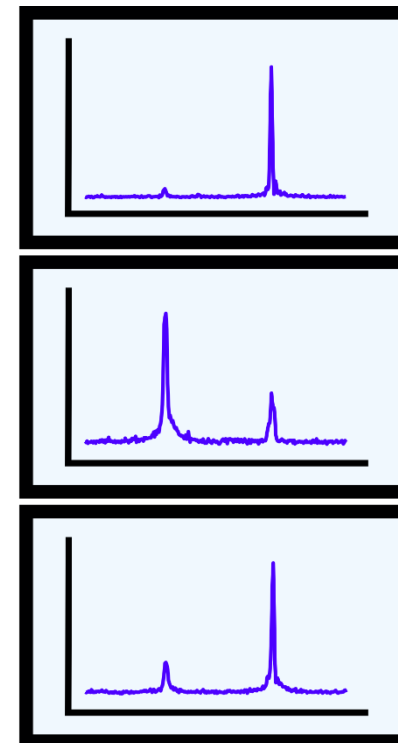


```
1 > RECPopDataDir > 2024_01_16_NCnKR > DataProcessingInference > BayesianInference > A_FunctionBayesNet.j
2 Function_restructDatInf(paths)
3
4 ##### OBSERVABLES #####
5
6 m = length(paths);
7
8 DataAll = Array{Any,1}(undef, m)
9
10 for i in 1:m
11     DataAll[i] = Matrix(CSV_read(paths[i], DataFrame));
12 end
13 stSIm = maximum([size(DataAll[i])[1] for i in 1:m]);
14 stS1 = reshape([size(DataAll[i])[1] for i in 1:m], 1, m);
15
16 obser = 2;
17 obSta = Array{Int,2}(undef, 1, 2)
18 obSta[1,:] = [1,2];
19
20 Means = Array{Float64,3}(undef, stSIm, m, obser);
21 Errors = Array{Float64,3}(undef, stSIm, m, obser);
22 stS = Array{Int,2}(undef, stSIm, m)*0
23 stS2 = Array{Int,2}(undef, stSIm, m)
24
25 YObs = Array{Float64,2}(undef, 3, m);
26 tml = maximum([length(DataAll[i][1,1]:DataAll[i][1,end,1]) for i in 1:m]);
27 ts = Array{Float64,2}(undef, tml, m);
28 ttp = Array{Float64,1}(undef, m);
29
30 ms = collect(2:2:obser*2);
31 for i in 1:m
32     stS[3:length(DataAll[i][1,1]:DataAll[i][1,end,1])] = convert{Int, DataAll[i][1,end,1]};
33     stS2[3:length(DataAll[i][1,1]:DataAll[i][1,end,1])] = convert{Int, DataAll[i][1,end,1]};
34     ts[1,i] = 1e-20;
35     for j in 1:obser
36         for k in 1:obser
```

## Microscopy Images



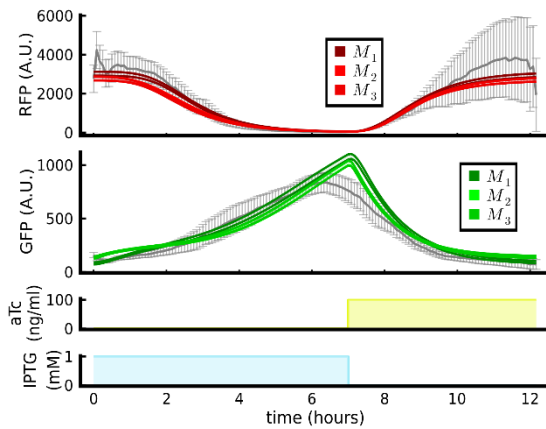
## Nuclear Magnetic Resonance Spectra



## Magnetic Resonance Images (MRI)

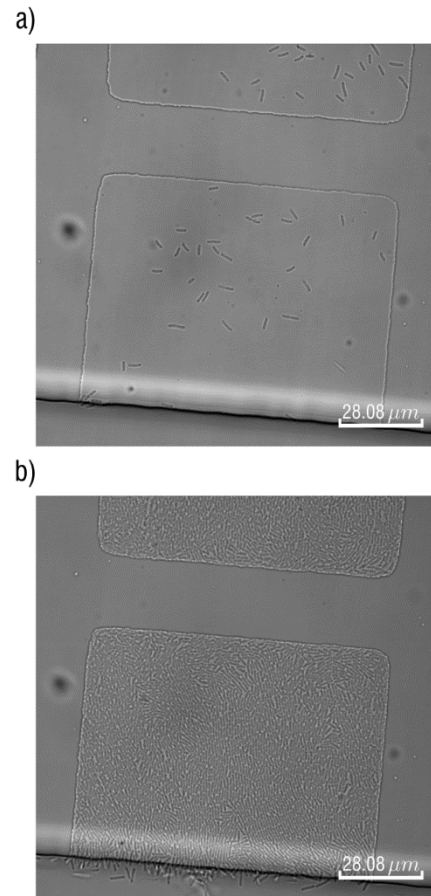
# My Datasets

## Computational Simulations and Scripts

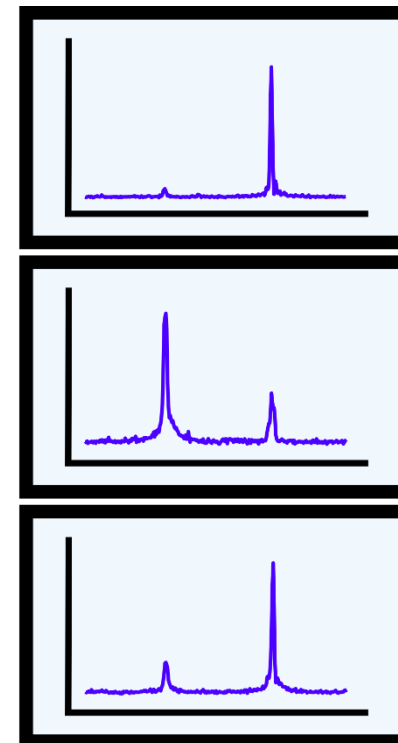


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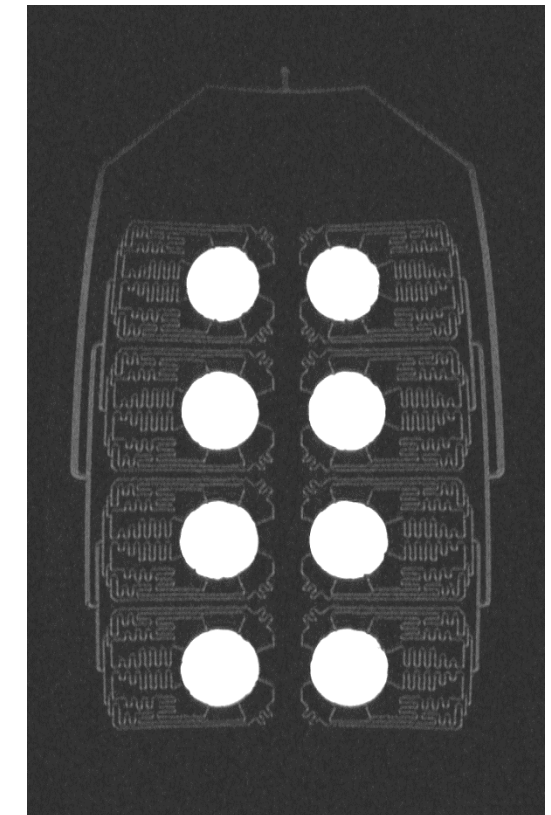
## Microscopy Images



## Nuclear Magnetic Resonance Spectra



## Magnetic Resonance Images (MRI)



# *During PhD*

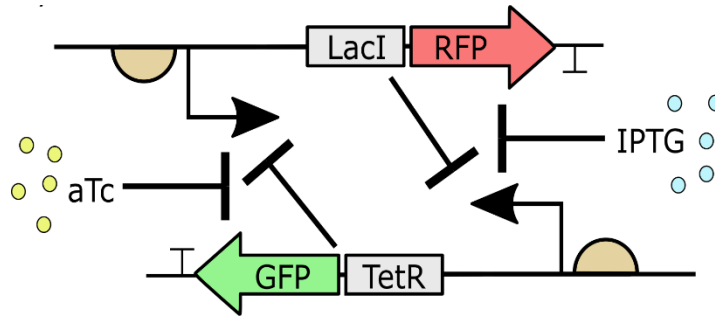


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# During PhD



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$$\frac{d[aTc]}{dt} = k_{aTc} (u_{aTc} - [aTc]) - g^P [aTc]$$

$$\frac{d[IPTG]}{dt} = k_{IPTG} (u_{IPTG} - [IPTG]) - g^P [IPTG].$$

$$P(\theta|D) = \frac{P(D|\theta) P(\theta)}{P(D)}$$

$$\frac{d[LacI]}{dt} = \frac{1}{g_L^m} \left( \kappa_L^{pm0} + \frac{\kappa_L^{pm}}{1 + \left( \frac{[TetR]}{\theta_{TetR}} \frac{1}{1 + \left( \frac{[aTc]}{\theta_{aTc}} \right)^{\eta_{aTc}}} \right)^{\eta_{TetR}}} \right) - g_L^P [LacI]$$

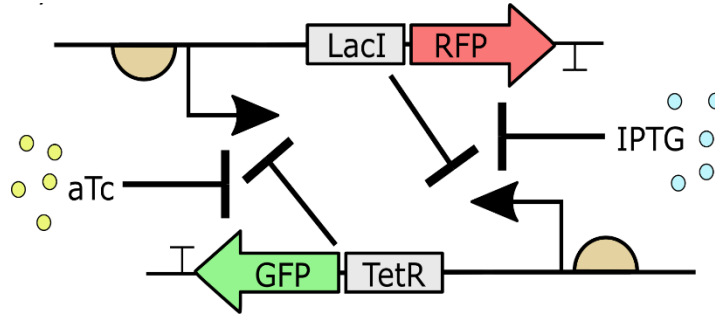
$$\frac{d[TetR]}{dt} = \frac{1}{g_T^m} \left( \kappa_T^{pm0} + \frac{\kappa_T^{pm}}{1 + \left( \frac{[LacI]}{\theta_{LacI}} \frac{1}{1 + \left( \frac{[IPTG]}{\theta_{IPTG}} \right)^{\eta_{IPTG}}} \right)^{\eta_{LacI}}} \right) - g_T^P [TetR],$$



# During PhD



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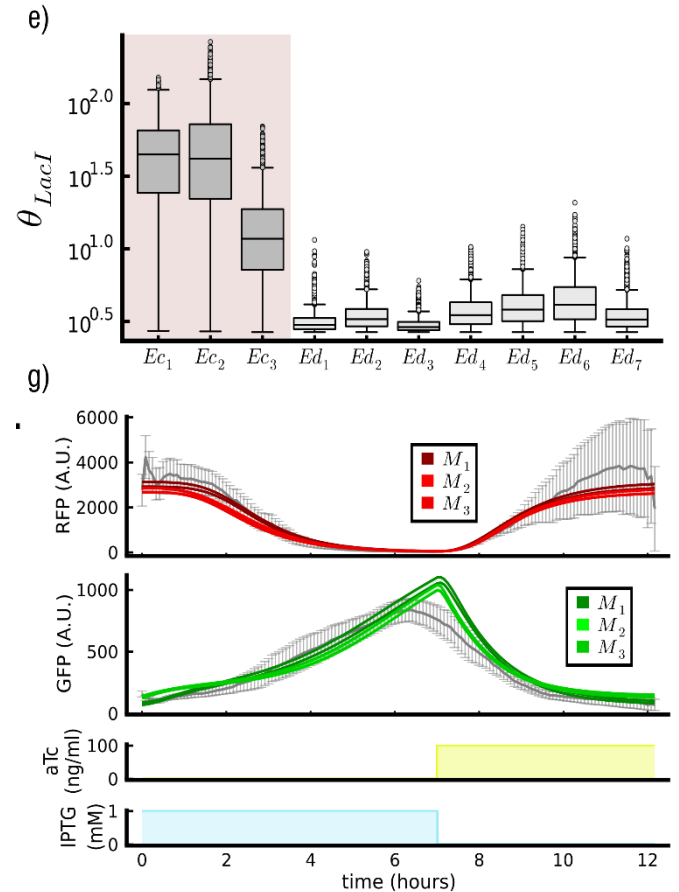
$$\frac{d[aTc]}{dt} = k_{aTc} (u_{aTc} - [aTc]) - g^P [aTc]$$

$$\frac{d[IPTG]}{dt} = k_{IPTG} (u_{IPTG} - [IPTG]) - g^P [IPTG].$$

$$P(\theta|D) = \frac{P(D|\theta) P(\theta)}{P(D)}$$

$$\frac{d[LacI]}{dt} = \frac{1}{g_L^m} \left( \kappa_L^{pm0} + \frac{\kappa_L^{pm}}{1 + \left( \frac{[TetR]}{\theta_{TetR}} \frac{1}{1 + \left( \frac{[aTc]}{\theta_{aTc}} \right)^{\eta_{aTc}}} \right)^{\eta_{TetR}}} \right) - g_L^P [LacI]$$

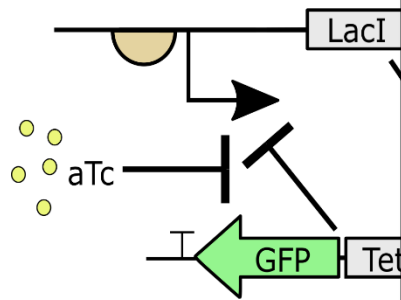
$$\frac{d[TetR]}{dt} = \frac{1}{g_T^m} \left( \kappa_T^{pm0} + \frac{\kappa_T^{pm}}{1 + \left( \frac{[LacI]}{\theta_{LacI}} \frac{1}{1 + \left( \frac{[IPTG]}{\theta_{IPTG}} \right)^{\eta_{IPTG}}} \right)^{\eta_{LacI}}} \right) - g_T^P [TetR],$$



# During PhD



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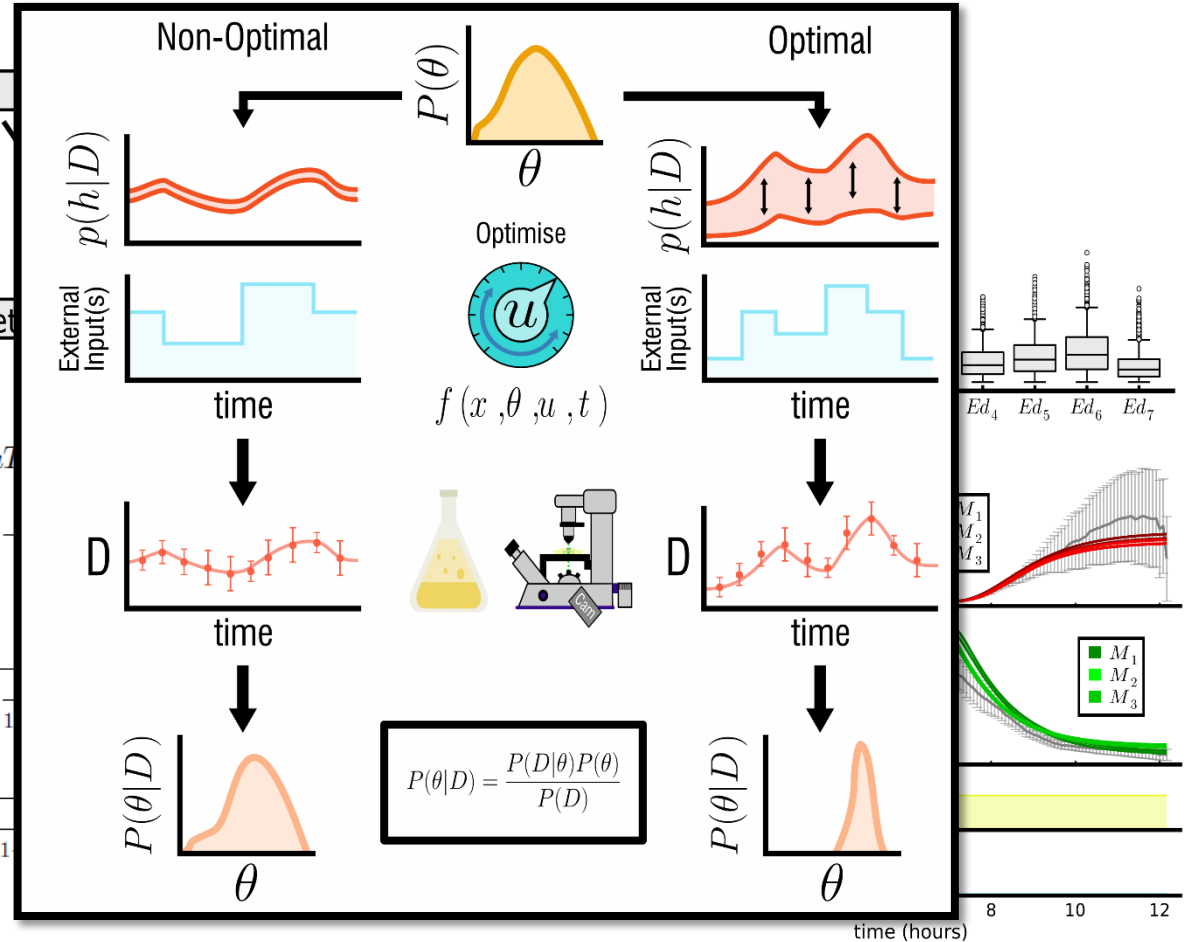
$$\frac{d[aTc]}{dt} = k_{aTc} (u_{aTc} - [aTc])$$

$$\frac{d[IPTG]}{dt} = k_{IPTG} (u_{IPTG} - [IPTG])$$

$$P(\theta|D) = \frac{P(D|\theta) P(\theta)}{P(D)}$$

$$\frac{d[LacI]}{dt} = \frac{1}{g_L^m} \left( \kappa_L^{pm0} + \frac{1}{1 + \left( \frac{[TetR]}{\theta_{TetR}} \right)^n} \right)$$

$$\frac{d[TetR]}{dt} = \frac{1}{g_T^m} \left( \kappa_T^{pm0} + \frac{1}{1 + \left( \frac{[LacI]}{\theta_{LacI}} \right)^n} \right)$$

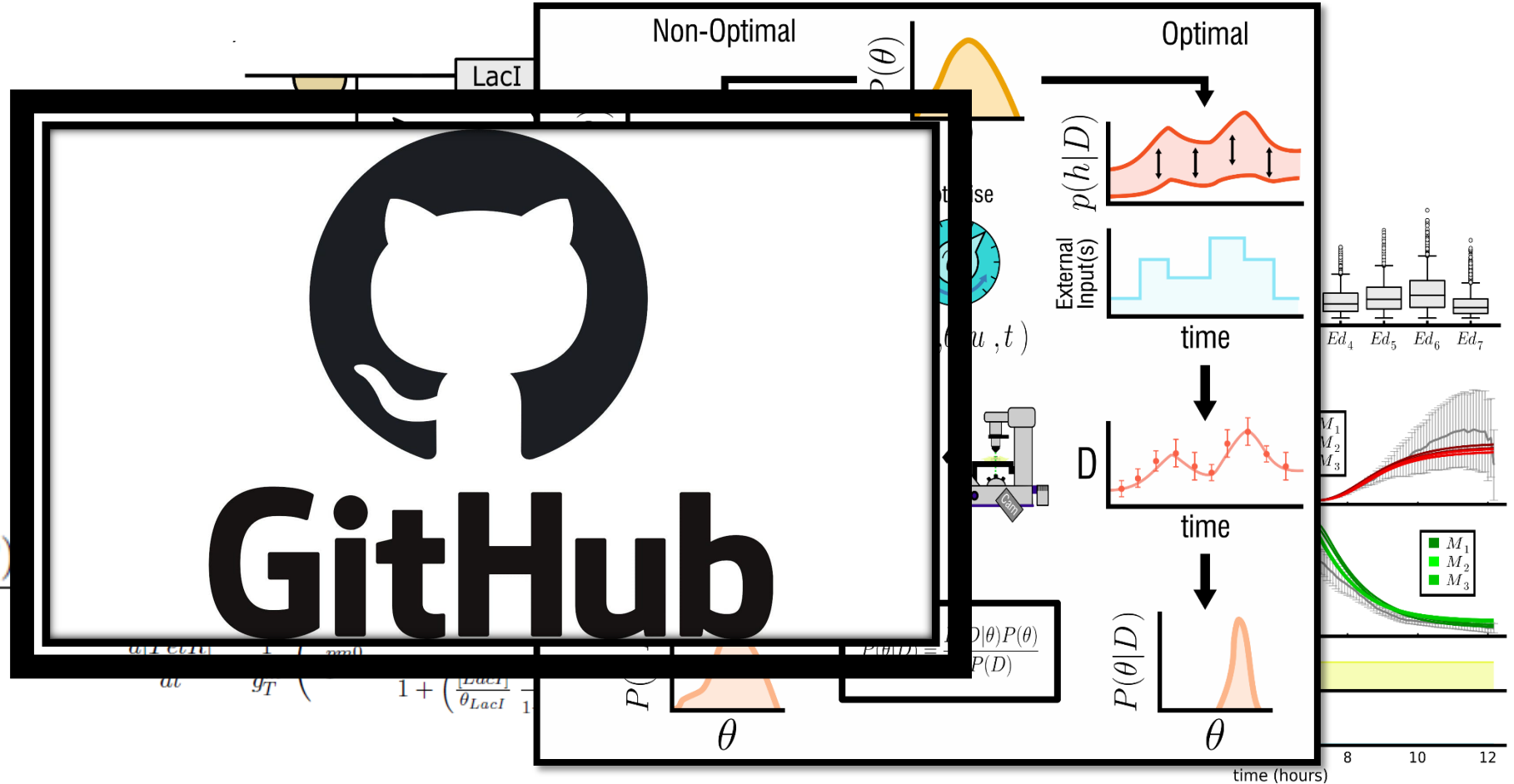


# During PhD

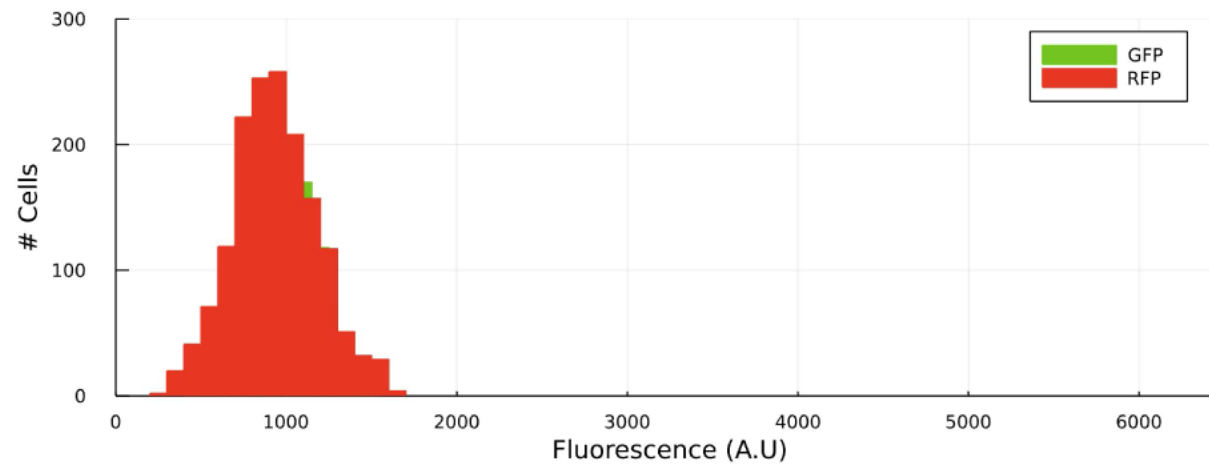
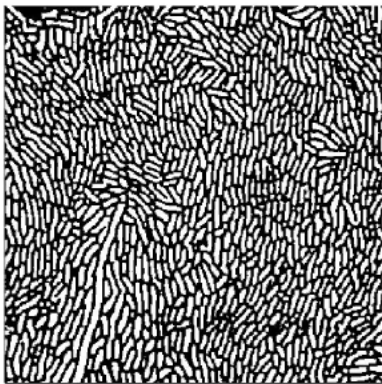
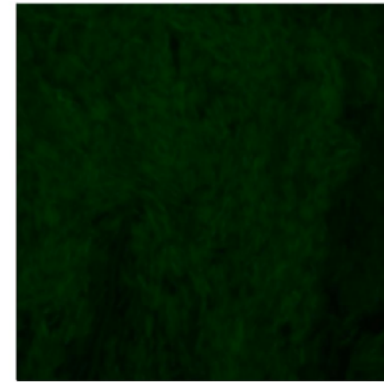
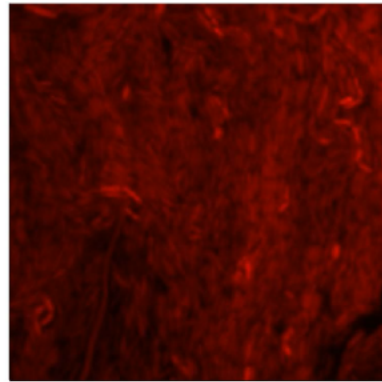
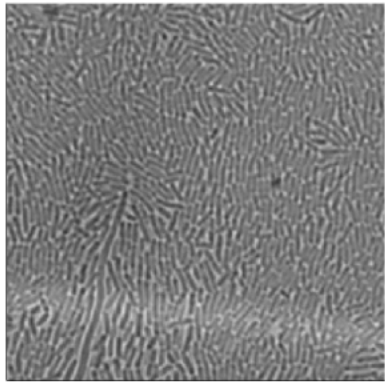


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$$P(\theta|D) = \frac{P(D|\theta) P(\theta)}{P(D)}$$

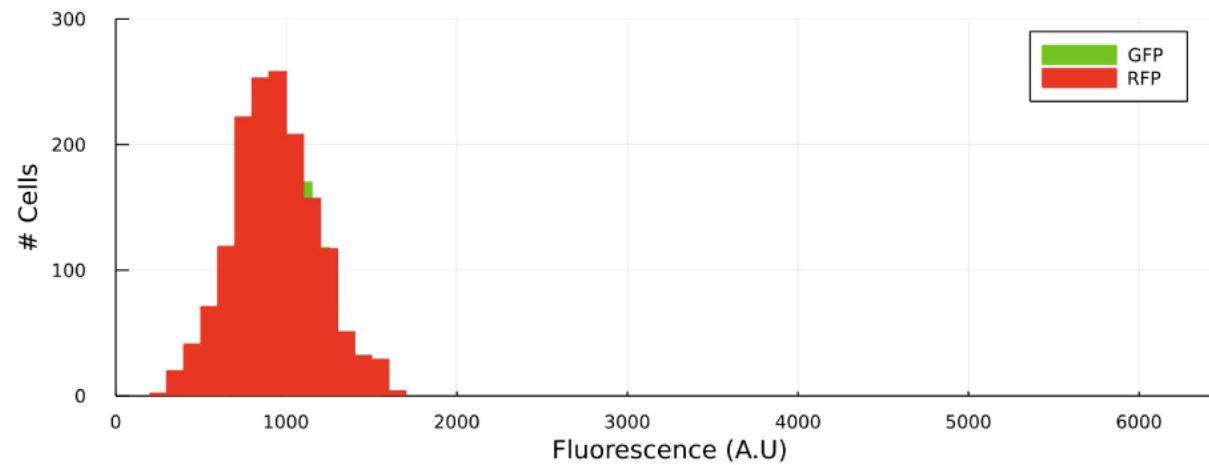
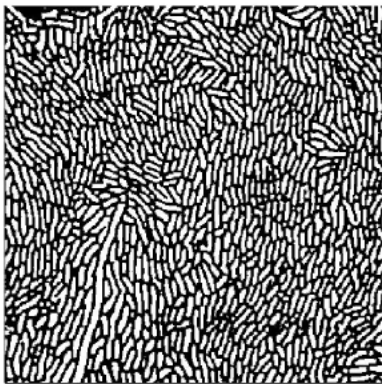
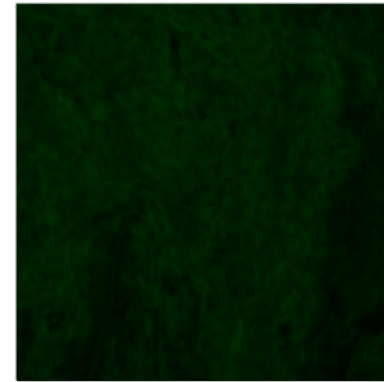
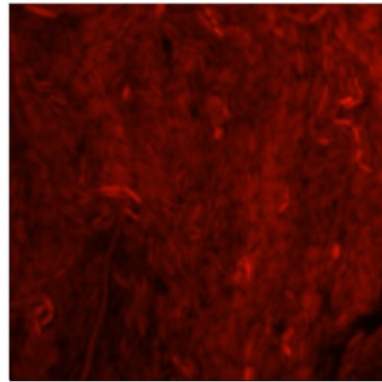
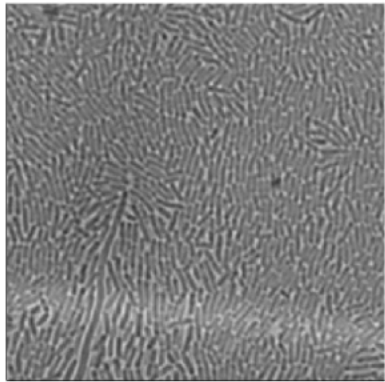


# *During PhD*



# *During PhD*

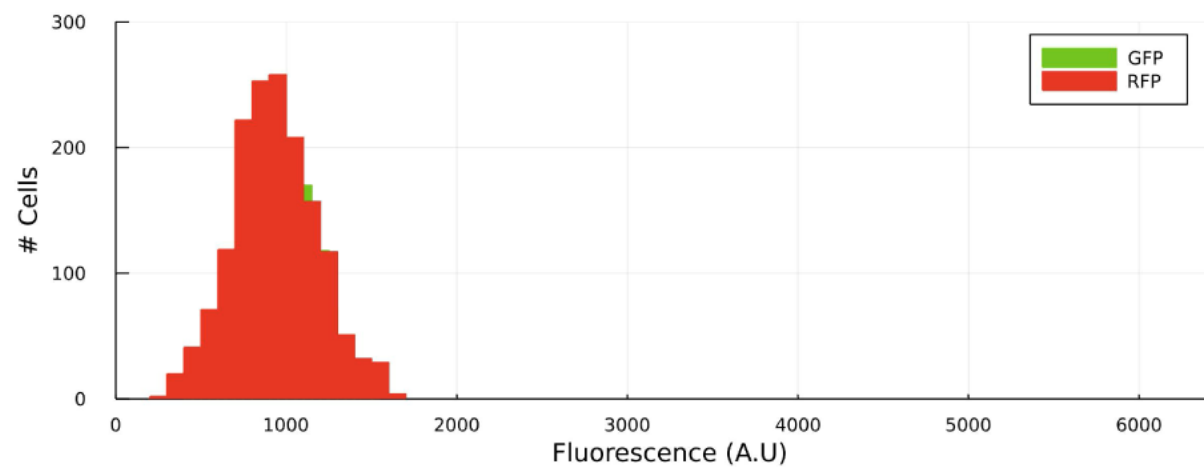
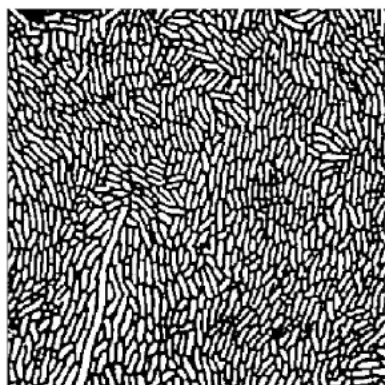
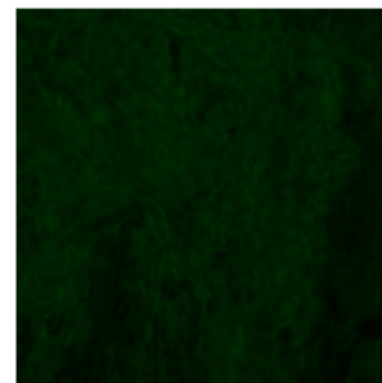
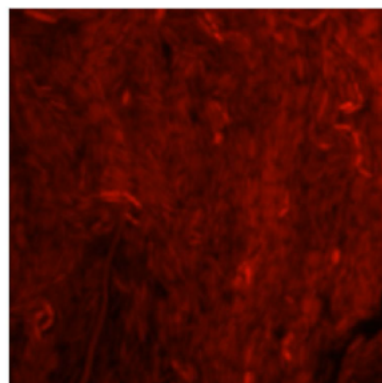
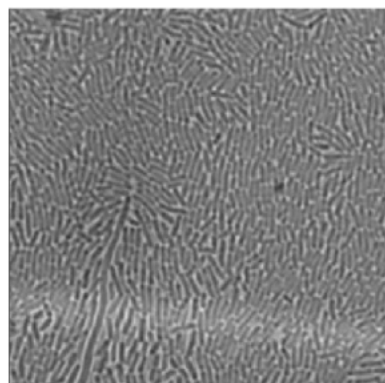
3 channels \* 8 Positions \* Acquisition Every 5 min for 48 hours = 13824 per experiment



# *During PhD*

3 channels \* 8 Positions \* Acquisition Every 5 min for 48 hours = 13824 per experiment

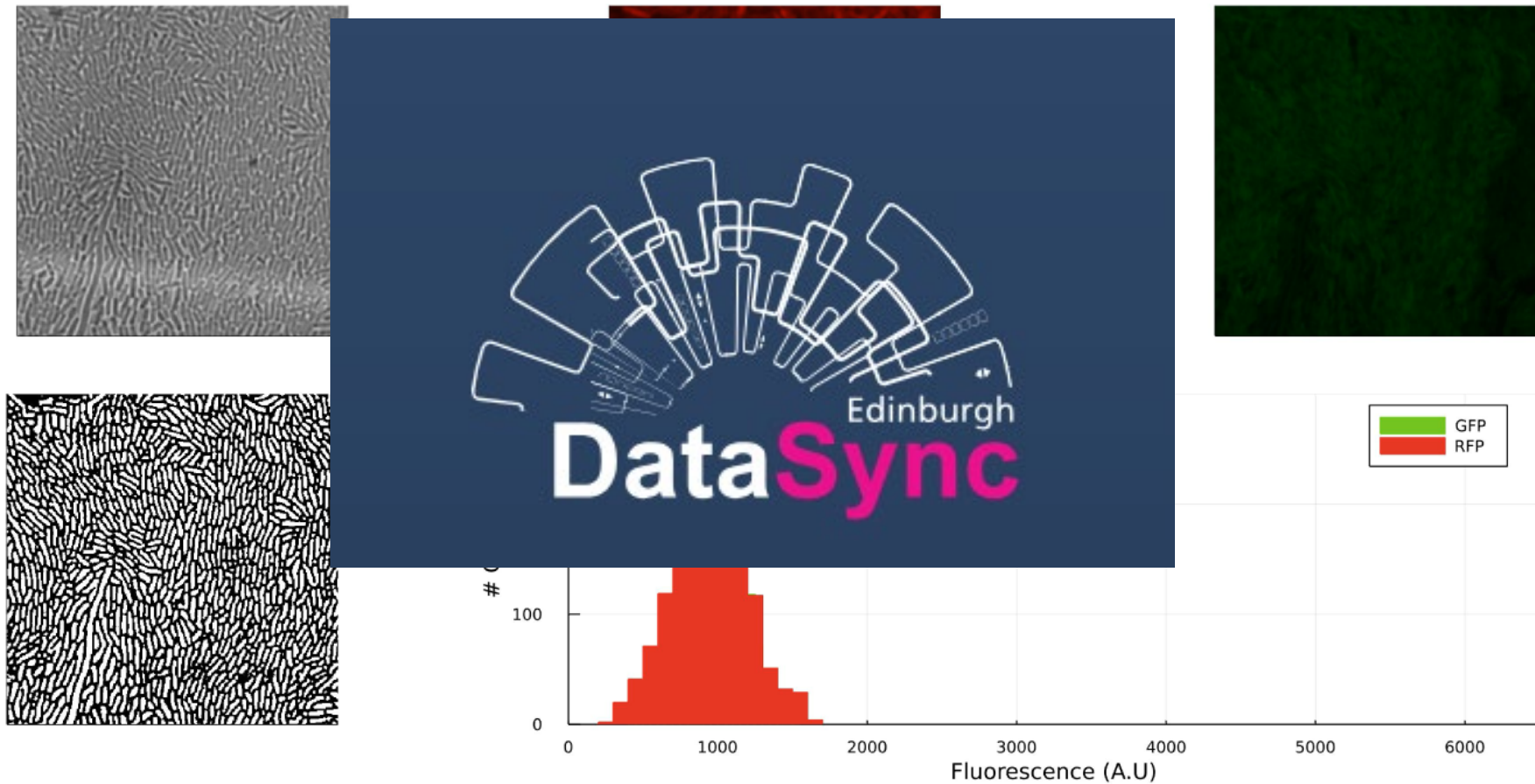
Plus, an automated segmentation mask per image!!!



# *During PhD*

3 channels \* 8 Positions \* Acquisition Every 5 min for 48 hours = 13824 per experiment

Plus, an automated segmentation mask per image!!!



# During PhD



DataSync

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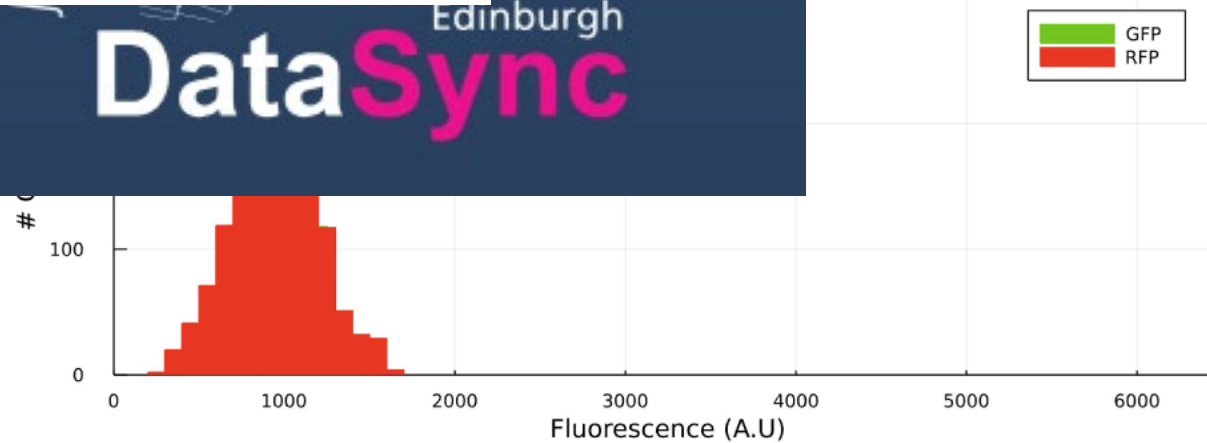
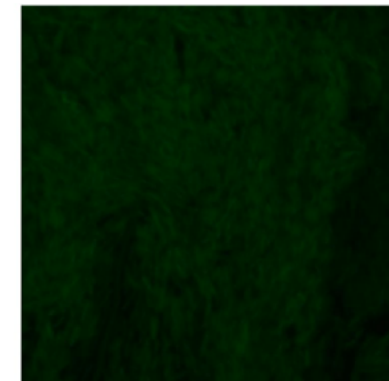
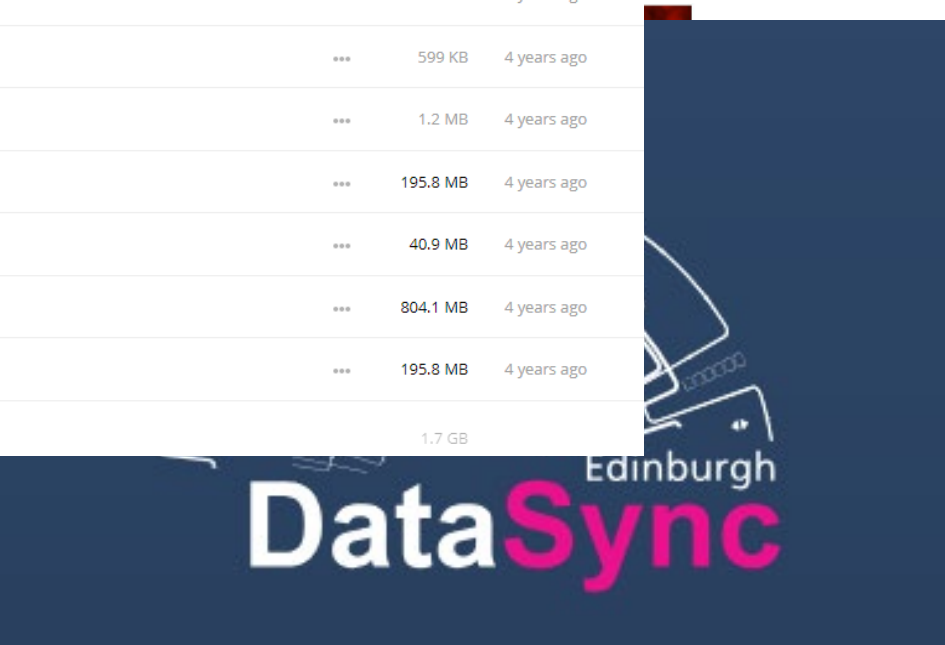
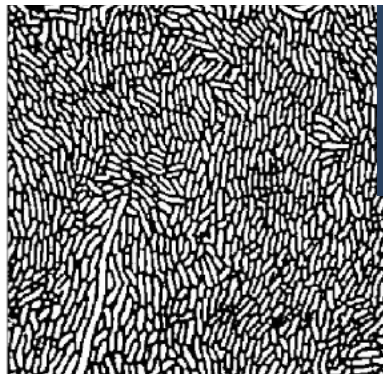
All files

Name	Size	Modified
Bayesian_MS	526.7 MB	4 years ago
Figure2_Data	13 MB	4 years ago
Figure3_Data	599 KB	4 years ago
Figure5_Data	1.2 MB	4 years ago
Figure6_Data	195.8 MB	4 years ago
FigureS1_Data	40.9 MB	4 years ago
Frequentist_MS	804.1 MB	4 years ago
Stability_Analysis	195.8 MB	4 years ago

8 folders 1.7 GB


or 48 hours = 13824 per experiment

n mask per image!!!





# During PhD

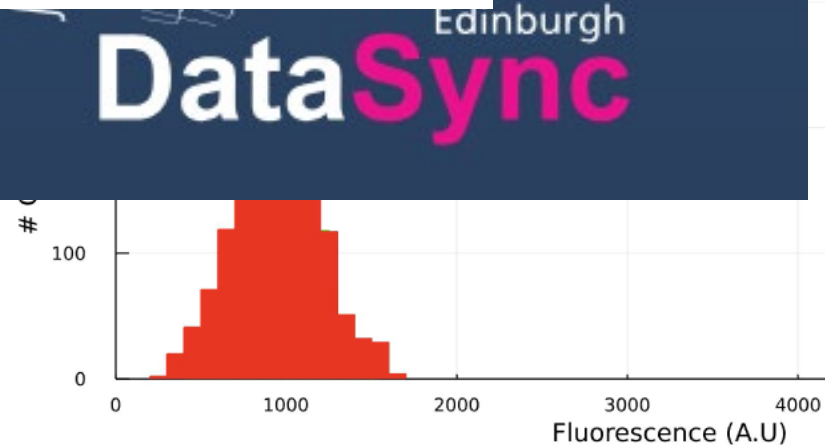
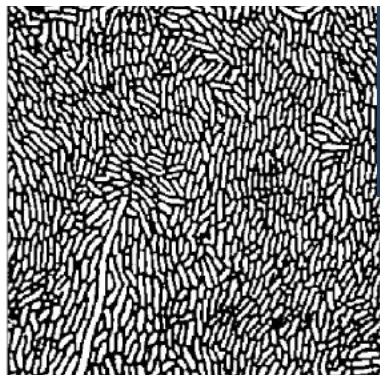


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FigureS1_Data	40.9 MB	4 years ago
Frequentist_MS	804.1 MB	4 years ago
Stability_Analysis	195.8 MB	4 years ago

8 folders 1.7 GB

or 48 hours = 13  
n mask per image



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DavidGomezC aa 59353a · 4 years ago 17 Commits

- Bayesian\_MS aa 4 years ago
- Frequentist\_MS Change directory name 4 years ago
- Images Update clean image scripts 4 years ago
- PriorShapeEffect InferenceScript 4 years ago
- Stability\_Analysis First push all scripts 4 years ago
- README.md Update README.md 4 years ago

### Optimally Designed Model Selection in Synthetic Biology

Here the scripts used to generate, analyse and visualise the data presented in the paper are made available.

The use of the scripts requires the RStan Package, available at the link:  
<https://cran.r-project.org/web/packages/rstan/index.html>

And the use of the Bayesian Optimisation package available at the link:  
<https://github.com/fmfn/BayesianOptimization>

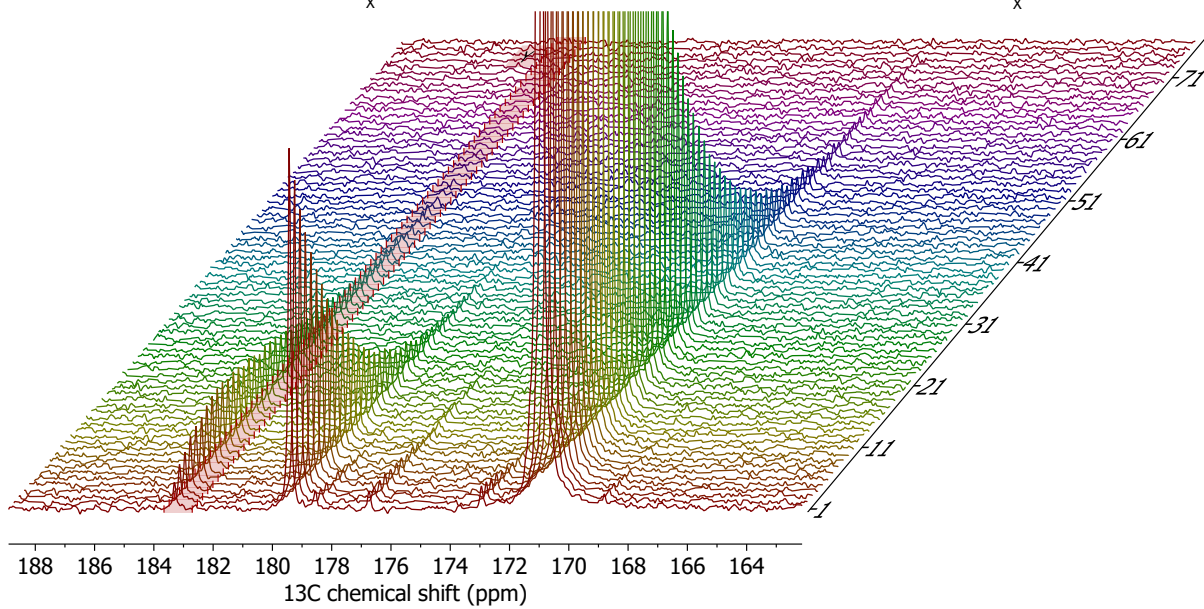
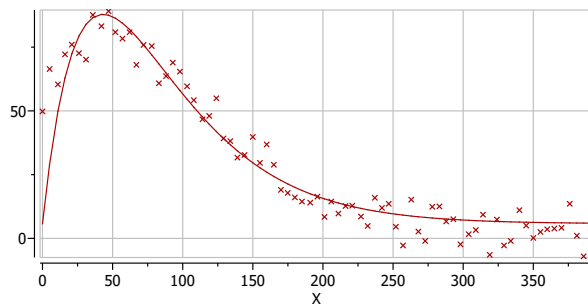
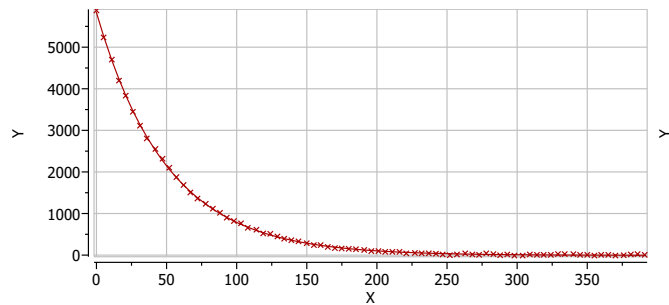
For the Matlab toolbox AMIGO2, refer to:  
<https://sites.google.com/site/amigo2toolbox/>

The data for the *Bayesian* case is organised in the following subfolders (Bayesian\_MS Directory):

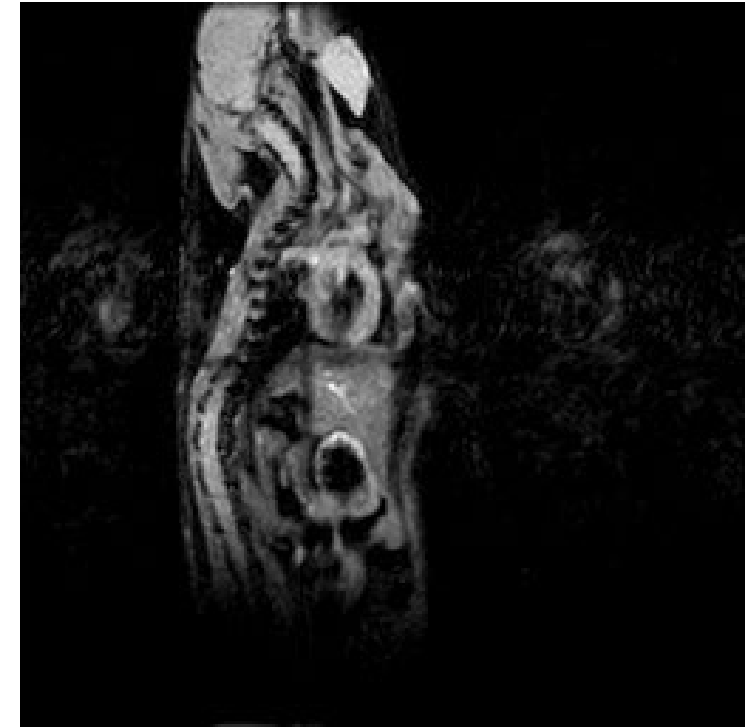
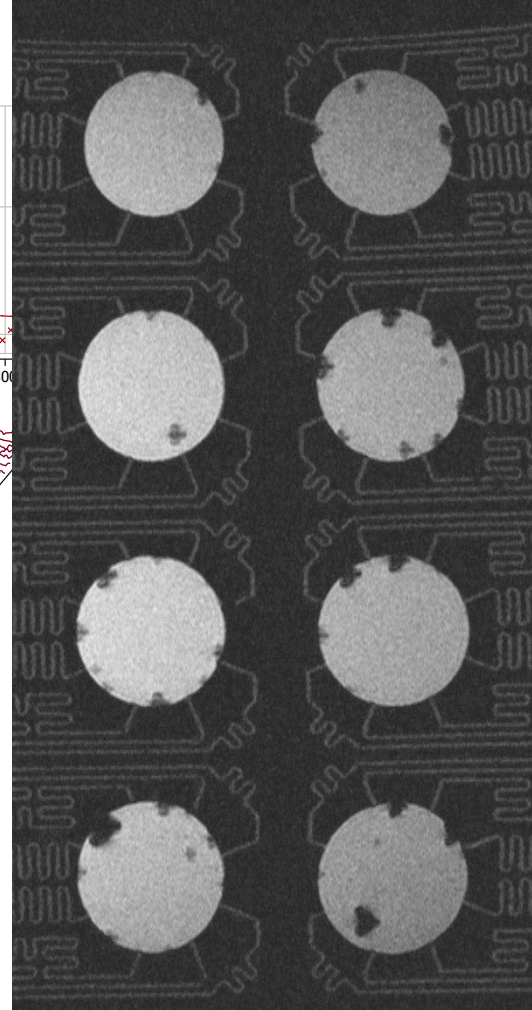
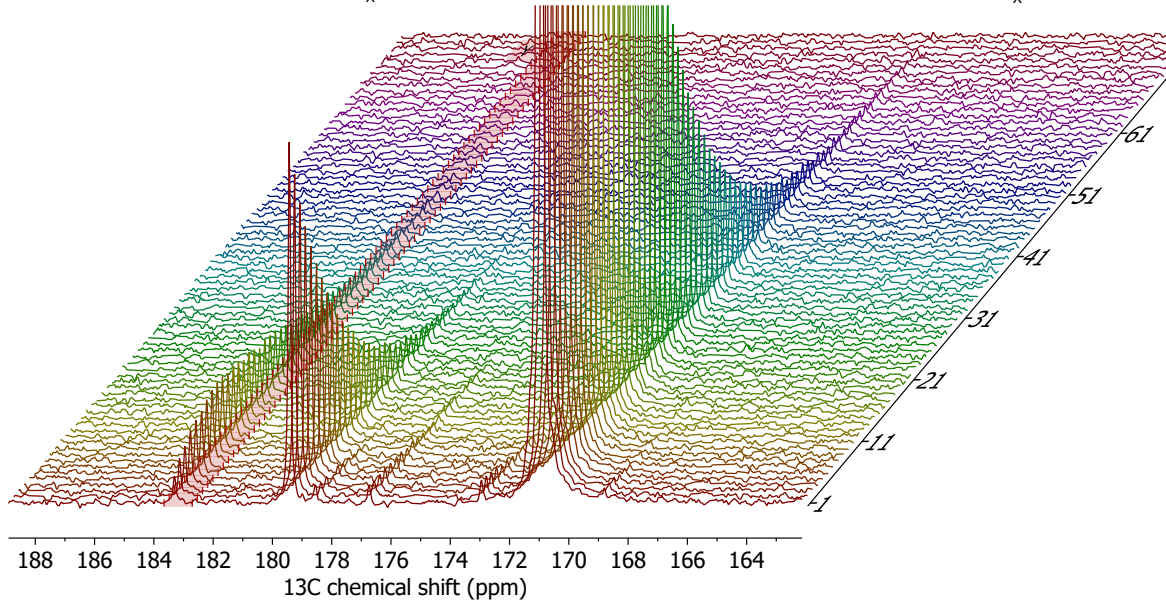
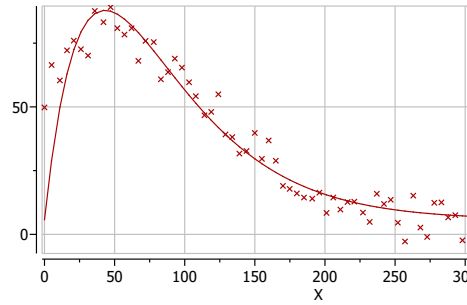
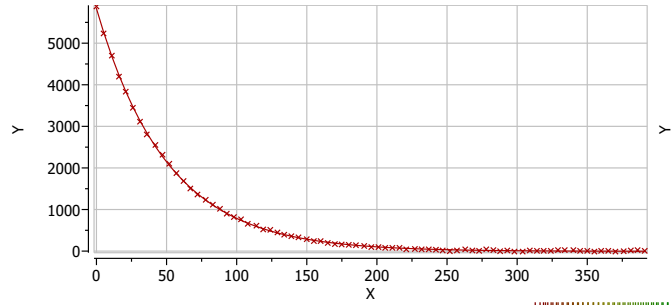
- Inference:
  - ODE\_Model1.stan*, stan statistical model script with Model 1 (M1) published by Lugagne *et al.*, used to perform Bayesian Inference of the experimental data from [1].
  - ODE\_Model2.stan*, stan statistical model script with Model 2 (M2) used to perform Bayesian Inference of the experimental data from [1].
  - ODE\_Model3.stan*, stan statistical model script with Model 3 (M3) used to perform Bayesian Inference of the experimental data from [1].
  - MultiExtractExp.R*, script designed to access the experimental data and experimental schemes from [1] to generate an appropriate list of objects to be passed to the stan model prior to the inference. The csv files are generated using the script DataExtraction.m.
  - DataExtraction.m*, script to extract the desired experimental data and experimental profiles from [1].
  - masterRun.R*, script to perform inference through RStan using the designed model *ODE\_Model.stan* and the list of data extracted from *MultiExtractExp.R*. The script allows performing inference on single datasets in series or on the combined set.
  - masterRunOptim.R*, script designed as the *masterRun.R* script but including an initial optimisation process for the initialisation of the 4 MCMC chains used in



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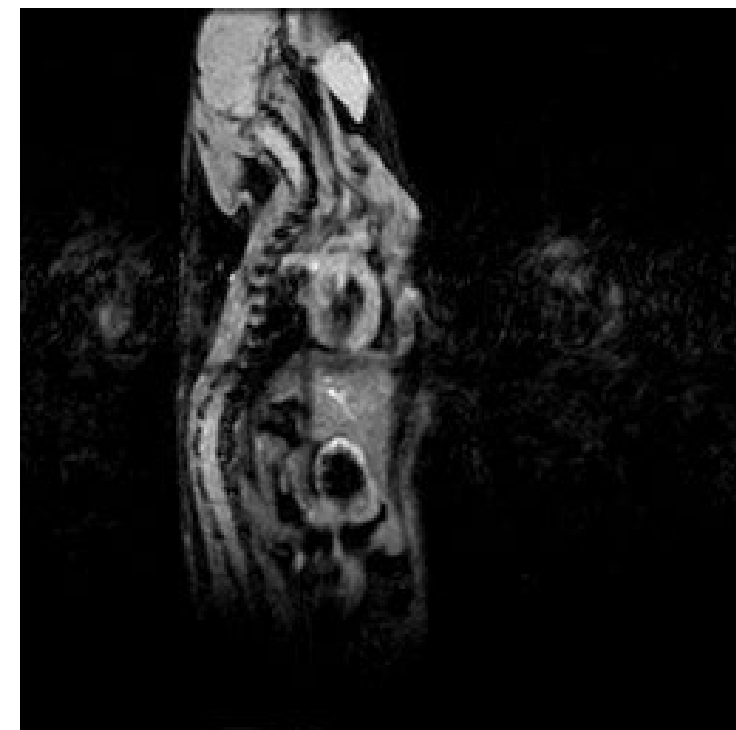
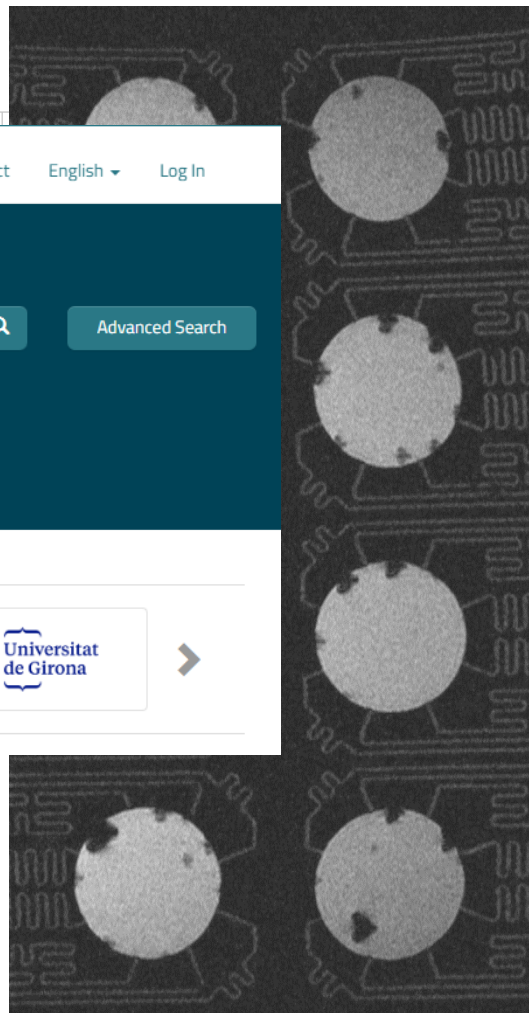
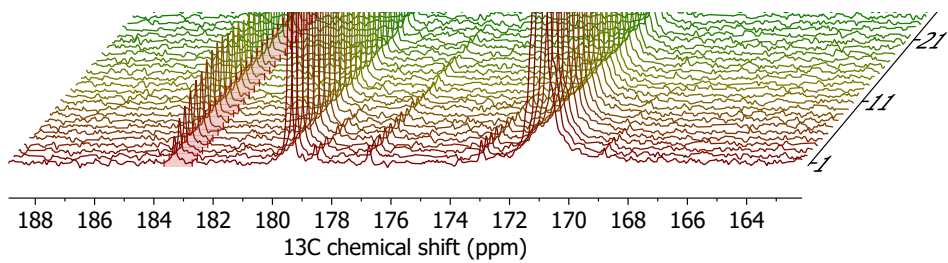
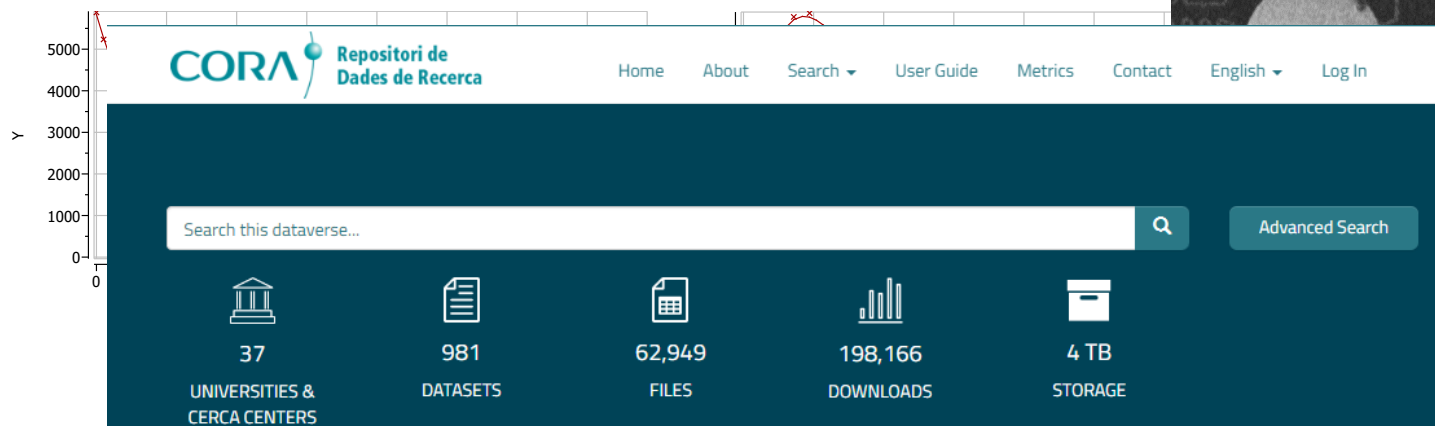


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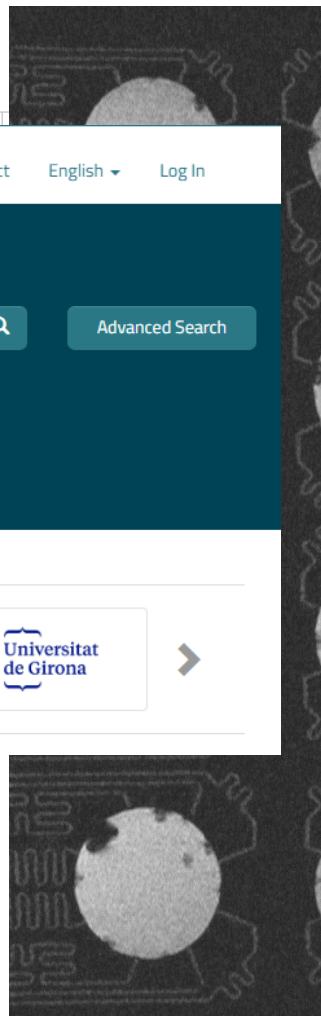
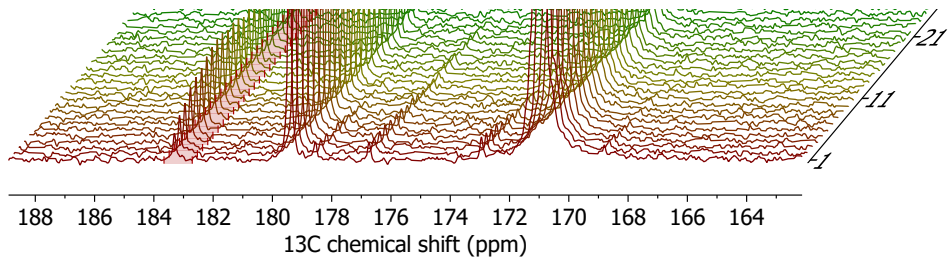


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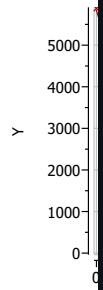
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- ▶ Diffusion\_hydrogel\_ependor
- ▶ Perffusion hydrogel
- ▼ Pump injection
  - ▶ PumpInjectionBoxPlots.png (41.1 KB)
  - ▶ PumpInjectionBoxPlots.svg (48.4 KB)
  - ▶ 19\_PreInject\_4
  - ▼ 20\_PostInject\_4
    - ▶ acqp (12.3 KB)
    - ▶ acqp.out (593 B)
    - ▶ AdjStatePerScan (1.1 KB)
    - ▶ configscan (5.8 KB)
    - ▶ Mask.png (170 B)
    - ▶ MaskBack.png (214 B)
    - ▶ method (18.6 KB)
    - ▶ pulseprogram.precomp (35.8 KB)
    - ▶ rawdata.job0 (73.1 KB)
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  - ▼ pdata
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      - ▶ 2dseq (48.0 KB)
      - ▶ id (536 B)
      - ▶ methreco (760 B)
      - ▶ MxiAcqReco.log (7.2 KB)
      - ▶ reco (11.1 KB)
      - ▶ reco.out (536 B)
      - ▶ visu\_pars (6.7 KB)
    - ▼ dicom
      - ▶ 4wellchip\_4wellchip\_Pump\_injection\_E20\_P1\_lm1.dcm (49.9 KB)
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  - ▶ 27\_PostInject\_5
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  - ▶ 30\_PostInject\_6
  - ▶ 31\_PreInject\_7
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  - ▶ MaskAll\_2.png (411 B)



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Combinations.ipynb	CleanScripts	6 months ago
DataProcessGen.ipynb	CleanScripts	6 months ago
DataProcessGenHydrogel.ipynb	CleanScripts	6 months ago
FastInjection.ipynb	CleanScripts	6 months ago
FitDiffusion.ipynb	Create FitDiffusion.ipynb	4 months ago
HydroGelPerfusion.ipynb	CleanScripts	6 months ago
PumpInjection.ipynb	CleanScripts	6 months ago
README.md	Update README.md	5 months ago

README

## ScaffoldsDifPerfPaper\_2023

This repository contains all the Python scripts developed to process the MRI data from the paper "Leveraging Magnetic Resonance Imaging to Study Biocompatible Scaffolds Perfusion for Lab-on-a-Chip Systems".

The MRI data generated and processed for this study can be found at <https://doi.org/10.34810/data1028>.

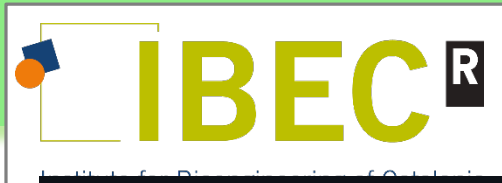
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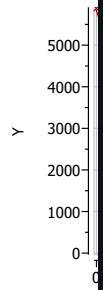
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- Perffusion hydrogel
- Pump injection
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- 19\_PreInject\_4
- 20\_PostInject\_4
  - acqp (12.3 KB)
  - acqp.out (593 B)
  - AdjStatePerScan (1.1 KB)
  - configscan (5.8 KB)
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  - MaskBack.png (214 B)
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- lists
- pdata
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  - dicom
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- 25\_PreInject\_5
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- 30\_PostInject\_6
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- 33\_PostInject\_7
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- 42\_PostInject\_8
- 48\_PreInject\_9
- 49\_PostInject\_9
- 00\_Readme.txt (4.0 KB)
- 20230724\_104854\_4wellchip\_MAR\_4wellchip\_scaffolddiffusionD20\_1\_1.zip (120.0 MB)
- DifussionCryogel.zip (80.8 MB)
- MaskAll.png (400 B)
- MaskAll\_2.png (411 B)





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Code

DavidGomezCabeza	Create FitDiffusion.ipynb	d6ab950 · 4 months ago	11 Commits
Combinations.ipynb	CleanScripts	6 months ago	
DataProcessGen.ipynb	CleanScripts	6 months ago	
DataProcessGenHydrogel.ipynb	CleanScripts	6 months ago	
FastInjection.ipynb	CleanScripts	6 months ago	
FitDiffusion.ipynb	Create FitDiffusion.ipynb	4 months ago	
HydroGelPerfusion.ipynb	CleanScripts	6 months ago	
PumpInjection.ipynb	CleanScripts	6 months ago	
README.md	Update README.md	5 months ago	

README

## ScaffoldsDifPerfPaper\_2023

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Files

- main
- Combinations.ipynb
- DataProcessGen.ipynb
- DataProcessGenHydrogel.ipynb
- FastInjection.ipynb
- FitDiffusion.ipynb
- HydroGelPerfusion.ipynb
- PumpInjection.ipynb
- README.md

ScaffoldsDifPerfPaper\_2023 / Combinations.ipynb

Preview Code Blame 1018 lines (1018 loc) · 303 KB

### Plot pixel sum

```
In [162]:
h = 1
for k in range(1,5):
    tm1 = dsPre[h][np.min(np.where(MPre[h]==k)[0]):np.max(np.where(MPre[h]==k)[0]), np.n
    tm2 = dsPre[h][np.min(np.where(MPost[h]==k)[0]):np.max(np.where(MPost[h]==k)[0]), np
    tm3 = dsPost[h][np.min(np.where(MPost[h]==k)[0]):np.max(np.where(MPost[h]==k)[0]), r
    tm4 = dsPost[h][np.min(np.where(MPre[h]==k)[0]):np.max(np.where(MPre[h]==k)[0]), np.

fig, axs = plt.subplots(dpi=150, figsize=(2,5))

mins = min(min(np.sum(tm1, 0)), min(np.sum(tm2, 0)), min(np.sum(tm3, 0)), min(np.sum
maxs = max(max(np.sum(tm1, 0)), max(np.sum(tm2, 0)), max(np.sum(tm3, 0)), max(np.sum

axs.plot(np.flip(np.concatenate((np.sum(tm2, 0), np.sum(tm1, 0))), range(len(np.cor
axs.plot(np.flip(np.concatenate((np.sum(tm3, 0), np.sum(tm4, 0))), range(len(np.cor
axs.set_xlabel('Pixel')
axs.set_ylabel('Pixel Intensity')

# axs.set_ylim(mins,maxs)
# axs.set_ylim(mins,maxs)

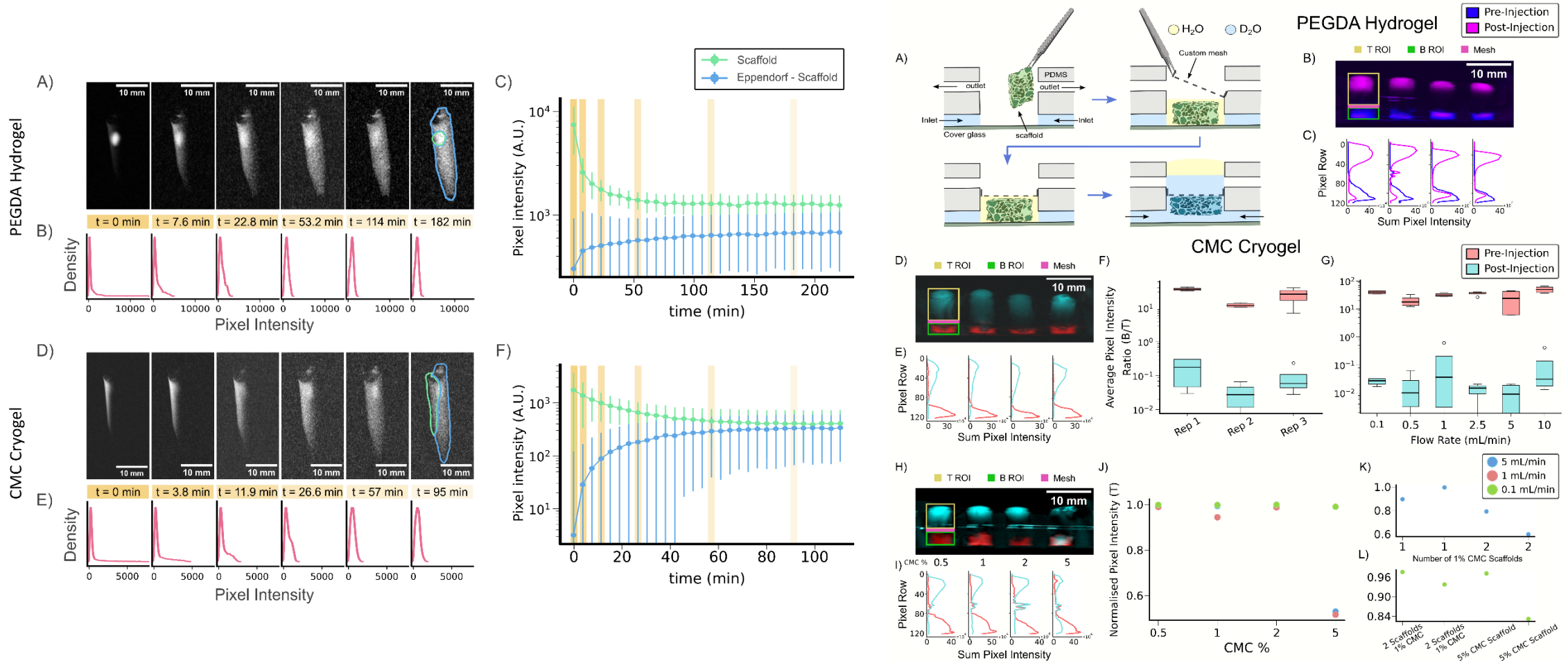
plt.savefig(patH+'/CMCPixelIntensity_Exper'+str(h+1)+'_Well'+str(k)+'.png')
plt.savefig(patH+'/CMCPixelIntensity_Exper'+str(h+1)+'_Well'+str(k)+'.svg')

plt.show()
```



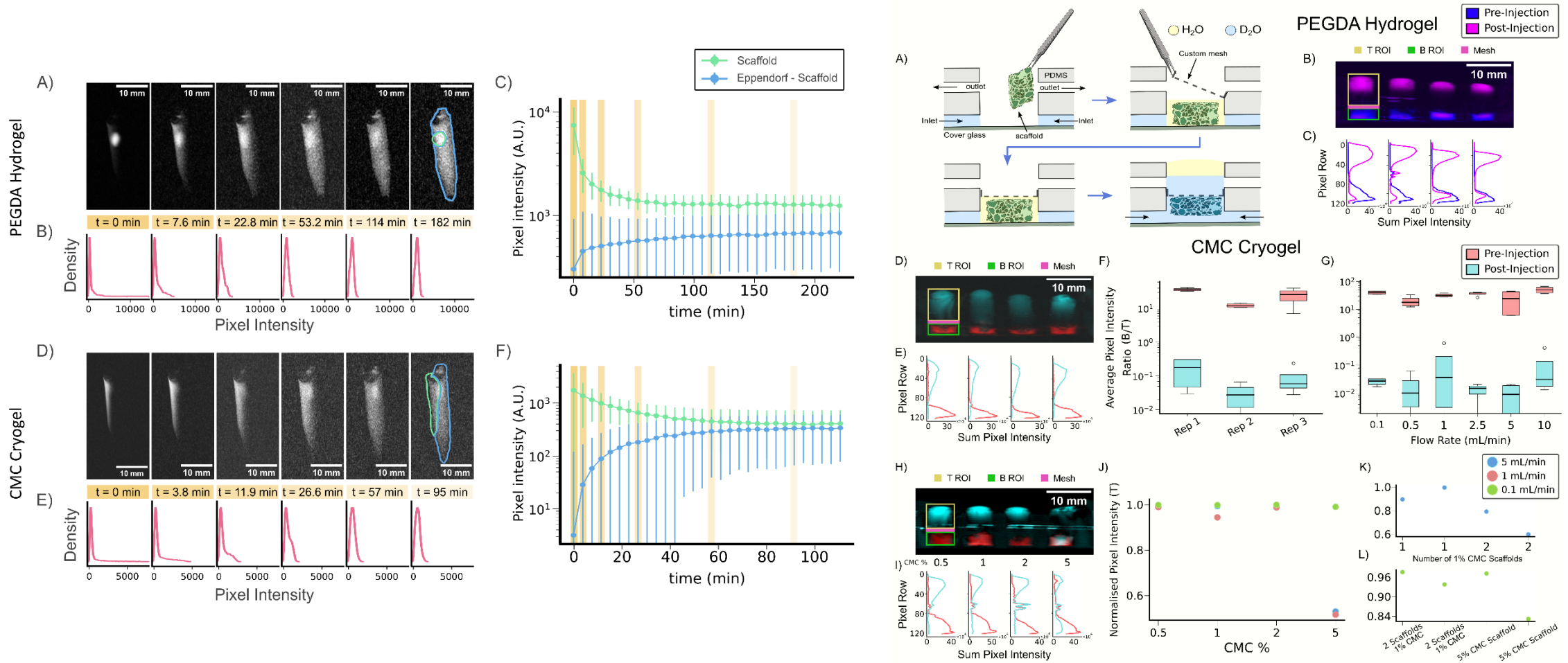
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The final figures are important



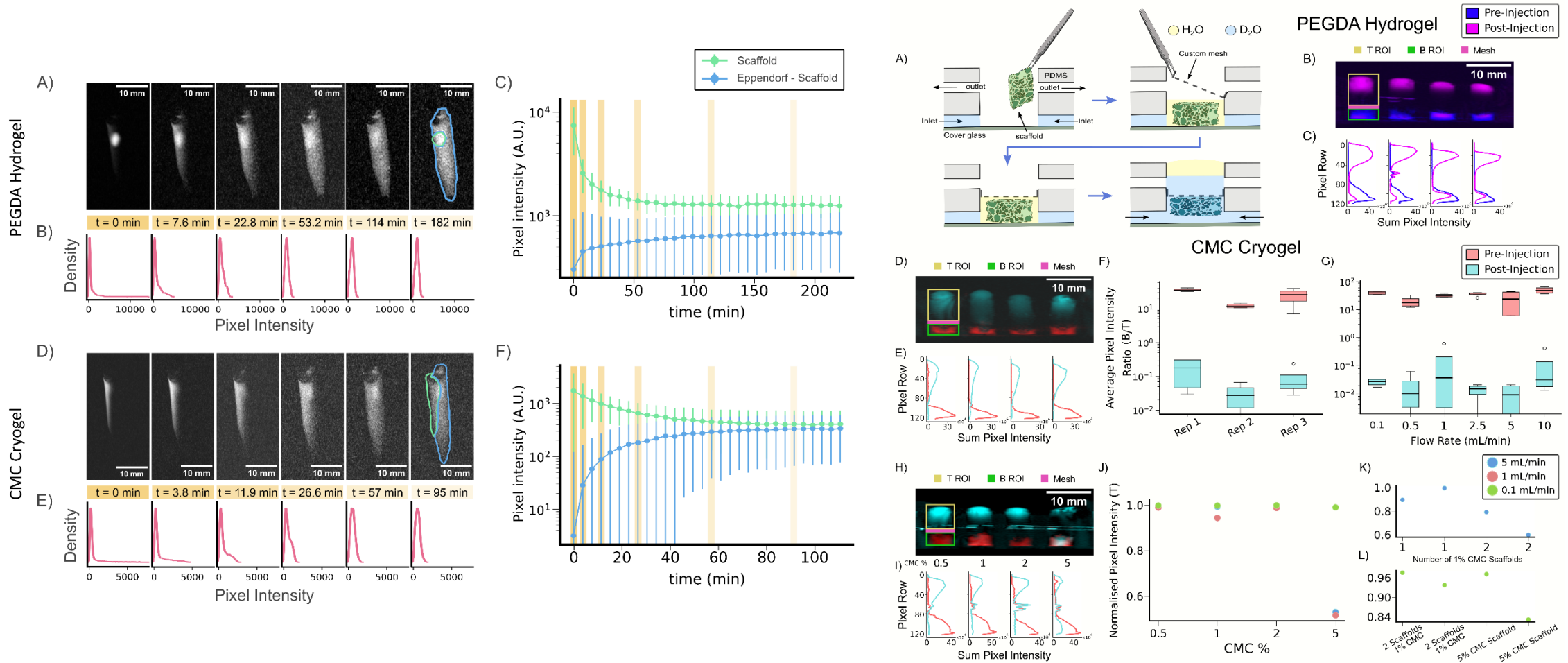
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The final figures are important, but so is the raw data



# Now As a Postdoc at IBEC

The final figures are important, but so is the raw data and the way we process this



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The final figures are important, but so is the raw data and the way we process this

