

FeCode_updated2025_inprogress_multiplates

2026-02-19

Things that need to be changed

```
Date_Run = "20260219"
plates<- c("Plate1", "Plate2", "Plate3")
Std_plates<- c("STD")
file_name<-"Experiment 1-4 Rerun"
Run_by = "Zoe Read">#Instrument user
Script_run_by ="Zoe Read"#Code user
Project = "TEMPEST"
Experiment="2025"
Run_notes=""#any notes from run

#Stds that should be excluded
stds_to_remove<-c("")
```

File paths

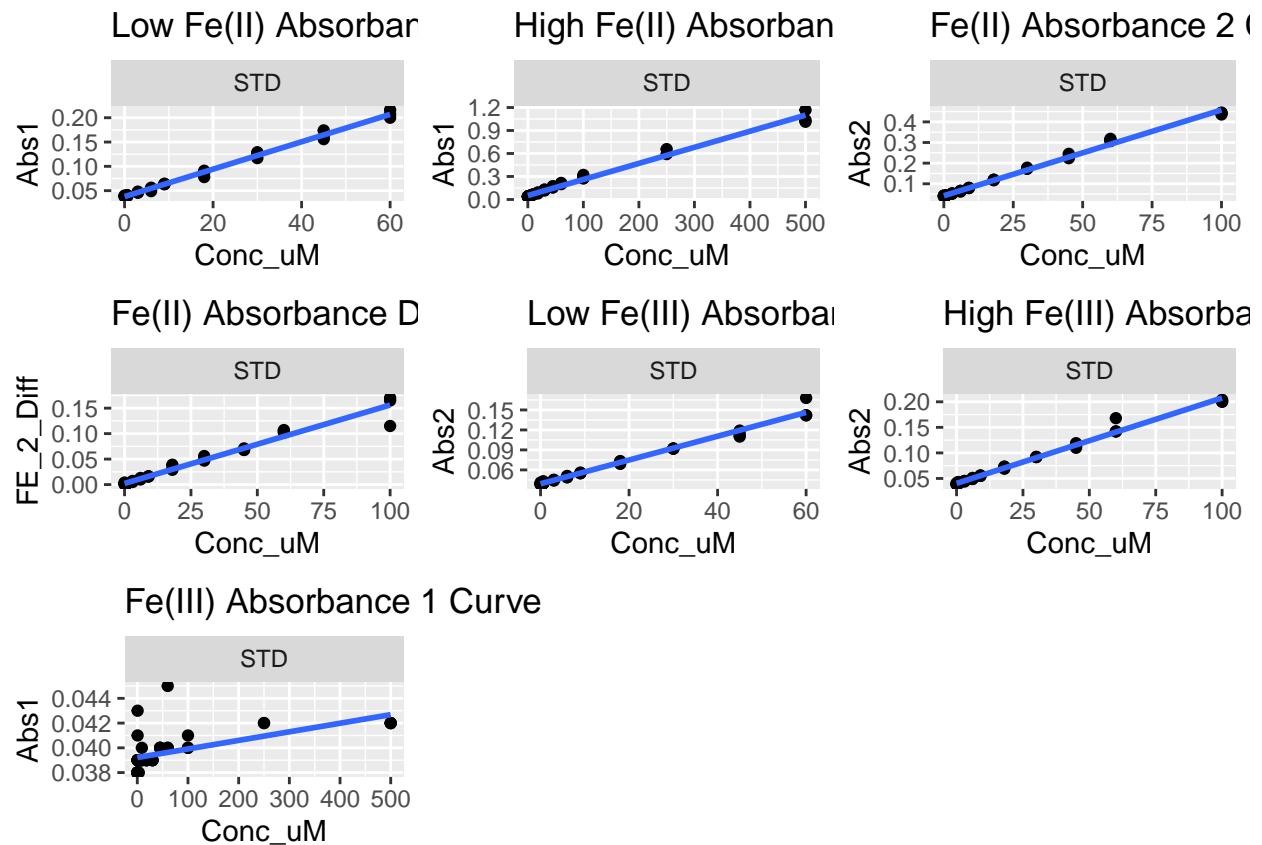
```
## [1] "Tidy Data/20260219_TEMPEST_Fe_STD.csv"

## [1] "Tidy Data/20260219_TEMPEST_Fe_Plate1.csv"
## [2] "Tidy Data/20260219_TEMPEST_Fe_Plate2.csv"
## [3] "Tidy Data/20260219_TEMPEST_Fe_Plate3.csv"
```

Plot standards

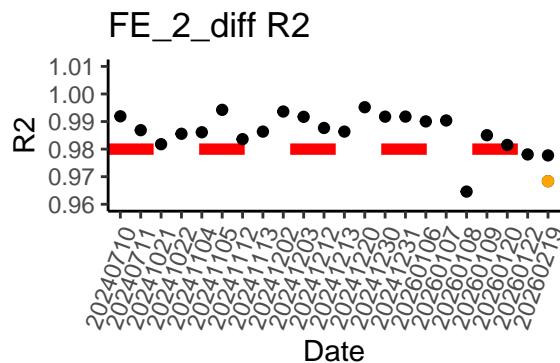
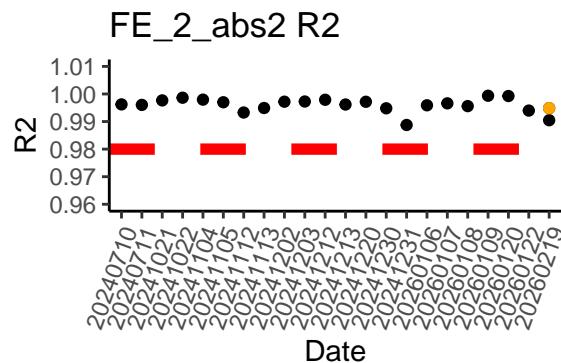
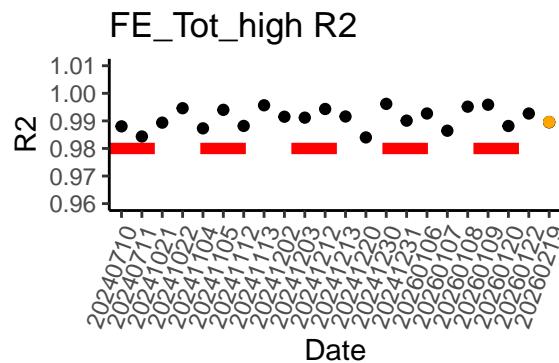
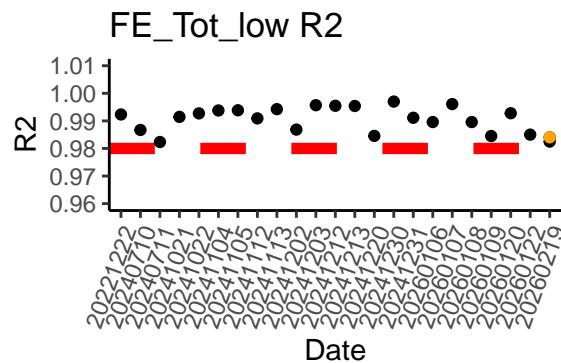
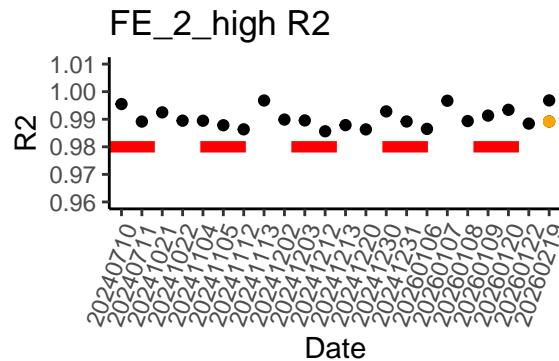
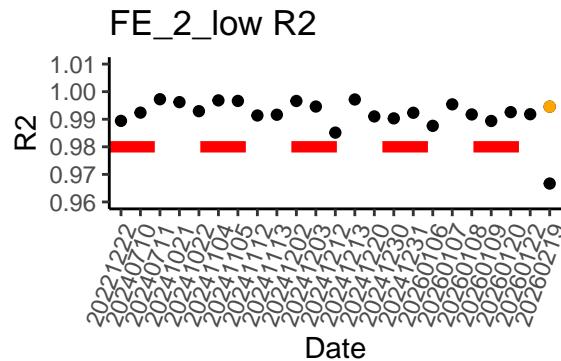
Table 1: Slopes

Date	Project	Curve	R2	Slope	Intercept	Top_STD
20260219	TEMPEST	FE_2_low	0.9945628	0.0028170	0.0378362	60
20260219	TEMPEST	FE_2_high	0.9891957	0.0020974	0.0515182	500
20260219	TEMPEST	FE_Tot_low	0.9840394	0.0017852	0.0391763	60
20260219	TEMPEST	FE_Tot_high	0.9895847	0.0016724	0.0403145	100
20260219	TEMPEST	FE_2_abs2	0.9948574	0.0041568	0.0421068	100
20260219	TEMPEST	FE_3_abs1	0.3357131	0.0000069	0.0392150	500
20260219	TEMPEST	FE_2_diff	0.9683687	0.0015394	0.0021925	100



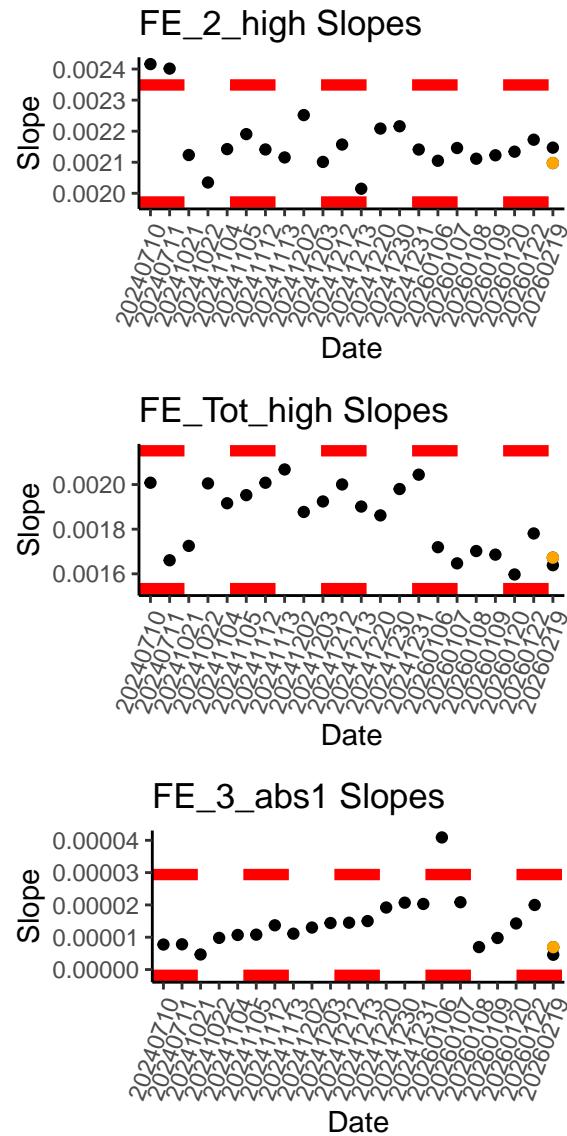
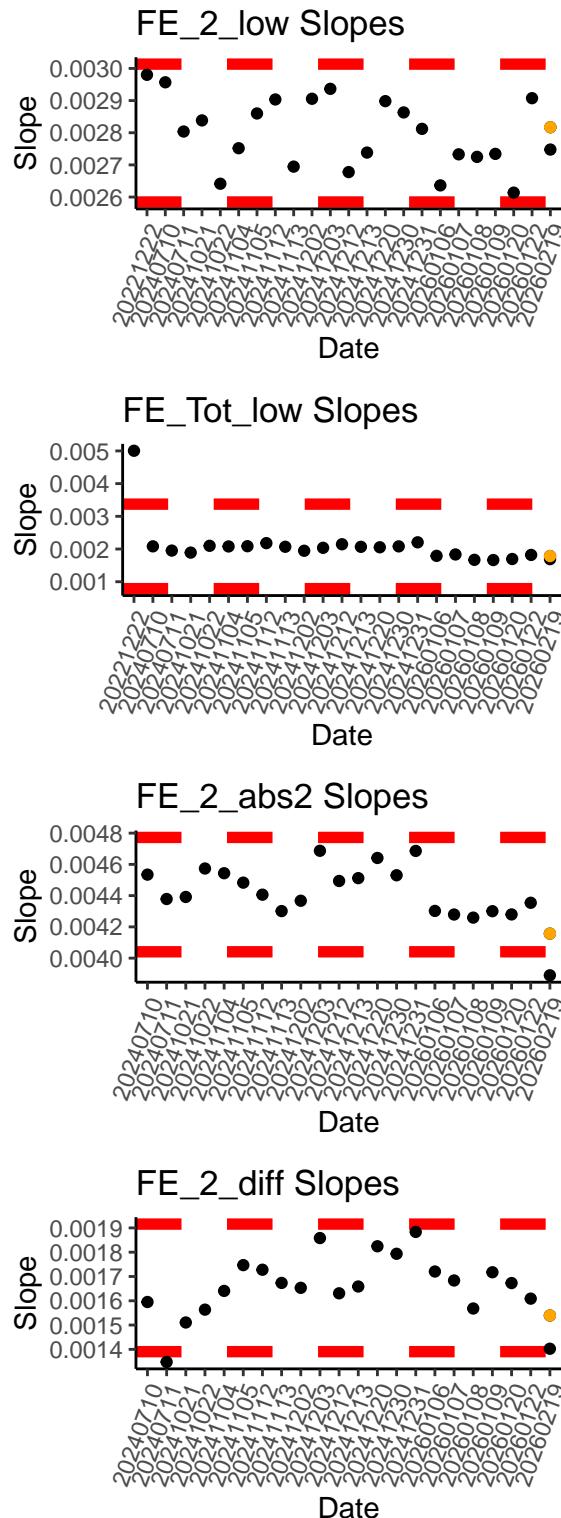
Checking STD Data against QAQC file

R2



```
## [1] "FE_2_low: Std Curve r2 GOOD"
## [1] "FE_2_high: Std Curve r2 GOOD"
## [1] "FE_Tot_low: Std Curve r2 is below cutoff! - REASSESS"
## [1] "FE_Tot_high: Std Curve r2 GOOD"
## [1] "FE_2_abs2: Std Curve r2 GOOD"
## [1] "FE_3_abs1: R2 will always be low"
## [1] "FE_2_diff: Std Curve r2 is below cutoff! - REASSESS"
```

Slopes



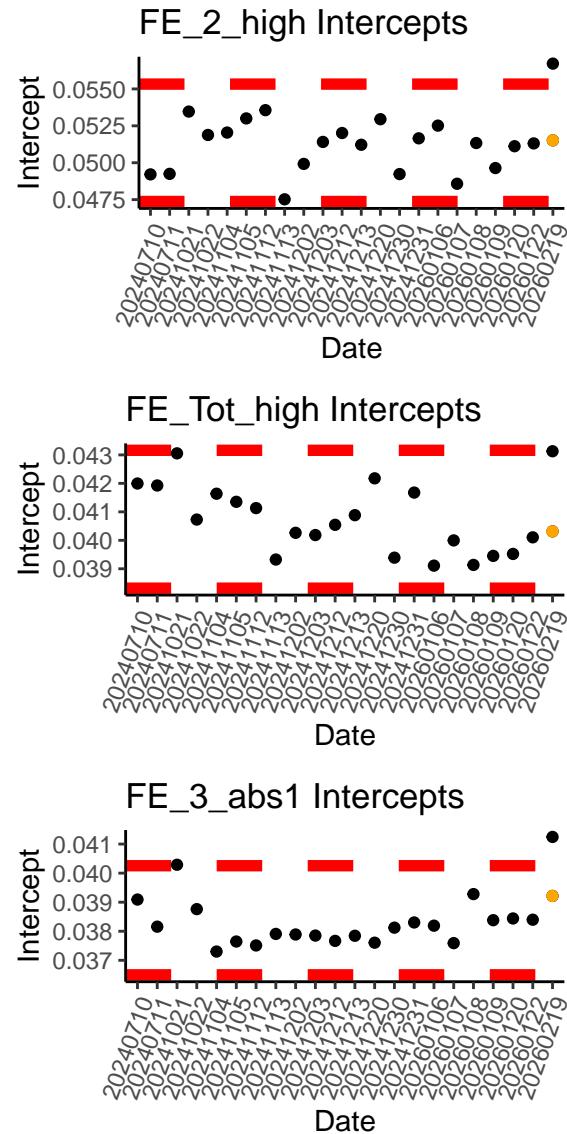
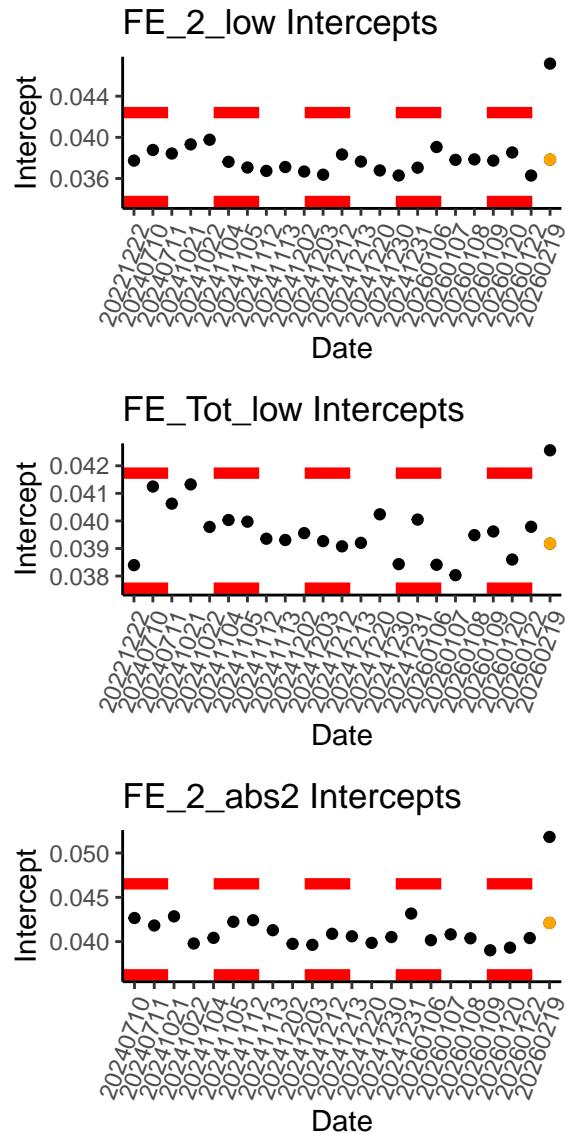
```
## [1] "FE_2_low:Std curve slope is with 2 sd of previous slopes"
## [1] "FE_2_high:Std curve slope is with 2 sd of previous slopes"
```

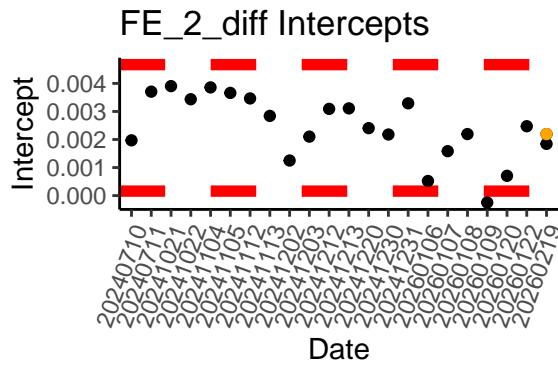
```

## [1] "FE_Tot_low:Std curve slope is with 2 sd of previous slopes"
## [1] "FE_Tot_high:Std curve slope is with 2 sd of previous slopes"
## [1] "FE_2_abs2:Std curve slope is with 2 sd of previous slopes"
## [1] "FE_3_abs1:Std curve slope is with 2 sd of previous slopes"
## [1] "FE_2_diff:Std curve slope is with 2 sd of previous slopes"

```

Intercepts



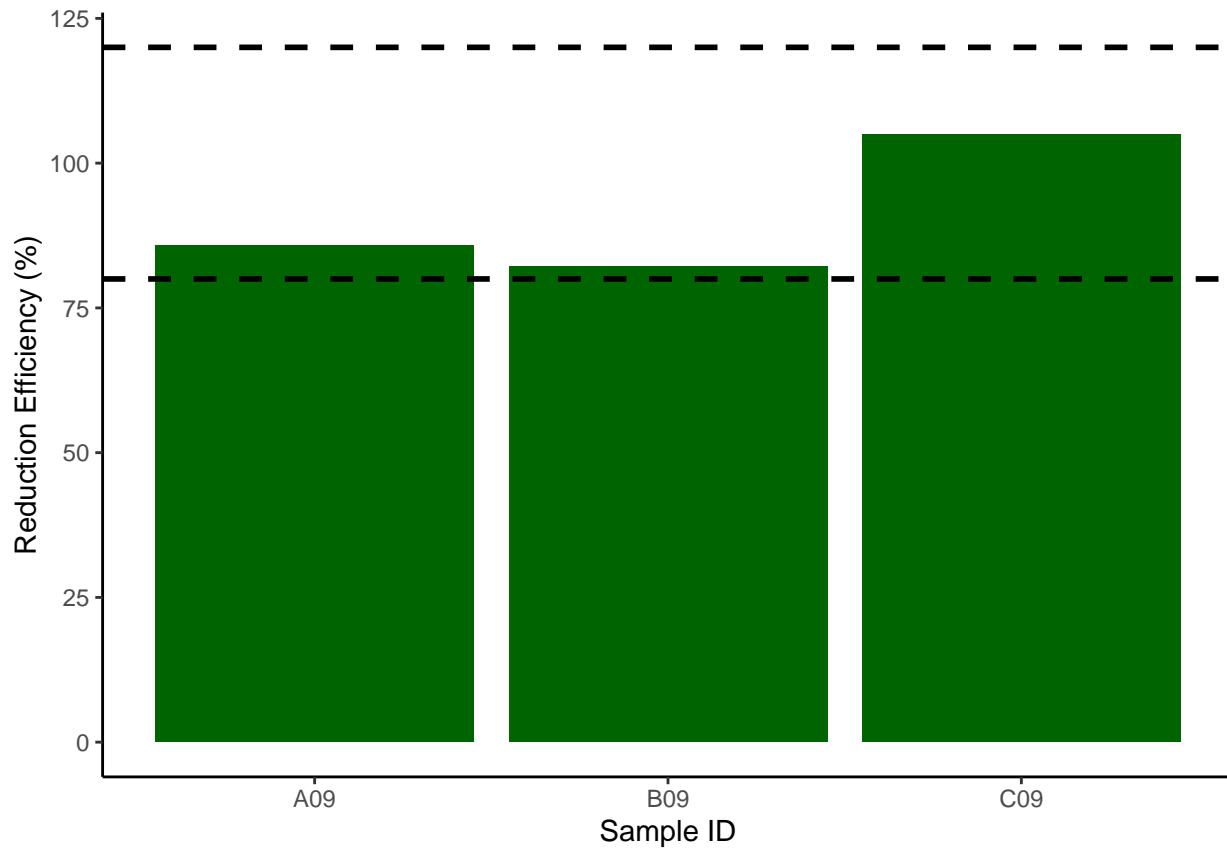


```
## [1] "FE_2_low:Std curve intercept is with 2 sd of previous intercepts"
## [1] "FE_2_high:Std curve intercept is with 2 sd of previous intercepts"
## [1] "FE_Tot_low:Std curve intercept is with 2 sd of previous intercepts"
## [1] "FE_Tot_high:Std curve intercept is with 2 sd of previous intercepts"
## [1] "FE_2_abs2:Std curve intercept is with 2 sd of previous intercepts"
## [1] "FE_3_abs1:Std curve intercept is with 2 sd of previous intercepts"
## [1] "FE_2_diff:Std curve intercept is with 2 sd of previous intercepts"
```

Calculate Reduction Efficiency

Table 2: Reduction Efficiency

ID	FE2	FE3	Eff	Eff1	Eff_flag
A09	0.207	0.142	68.59903	85.74879	OK
B09	0.216	0.142	65.74074	82.17593	OK
C09	0.200	0.168	84.00000	105.00000	OK



```
## [1] ">60% of Reduction Efficiencies are within range"
```

Method Minimum Detection Limit (MDL) Calculation

I use the lowest standard to calculate MDL How to calculate MDL https://www.epa.gov/sites/default/files/2016-12/documents/mdl-procedure_rev2_12-13-2016.pdf Look at Table 1 on page 5 The Student's t-value used to calculate the method detection limit (MDL) is the one appropriate for a 99% confidence level and a standard deviation estimate with n-1 degrees of freedom

```
## [1] 0.0008333078
```

Check standards QAQC

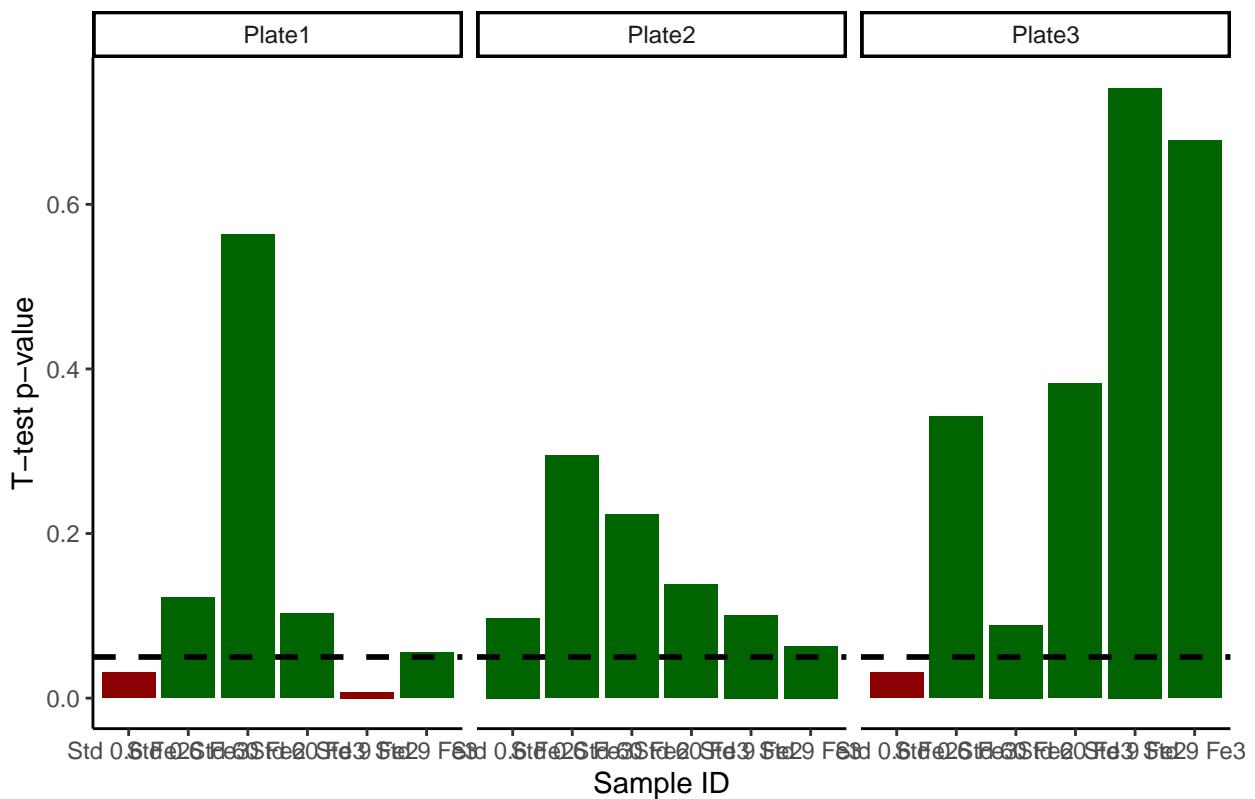
```
## [1] "Plate1"
## [1] "Fe2 Chk Std 0.6 is significantly different from Std - REASSESS"
## [1] "Fe2 Chk Std 9 is significantly different from Std - REASSESS"
## [1] "Fe2 Chk Std 60 GOOD"
## [1] "Fe 3 Chk Std 0.6 Fe2 GOOD"
## [1] "Fe 3 Chk Std 9 GOOD"
## [1] "Fe 3 Chk Std 60 GOOD"
## [1] "Plate2"
## [1] "Fe2 Chk Std 0.6 GOOD"
## [1] "Fe2 Chk Std 9 GOOD"
```

```

## [1] "Fe2 Chk Std 60 GOOD"
## [1] "Fe 3 Chk Std 0.6 Fe2 GOOD"
## [1] "Fe 3 Chk Std 9 GOOD"
## [1] "Fe 3 Chk Std 60 GOOD"
## [1] "Plate3"
## [1] "Fe2 Chk Std 0.6 is significantly different from Std - REASSESS"
## [1] "Fe2 Chk Std 9 GOOD"
## [1] "Fe2 Chk Std 60 GOOD"
## [1] "Fe 3 Chk Std 0.6 Fe2 GOOD"
## [1] "Fe 3 Chk Std 9 GOOD"
## [1] "Fe 3 Chk Std 60 GOOD"

```

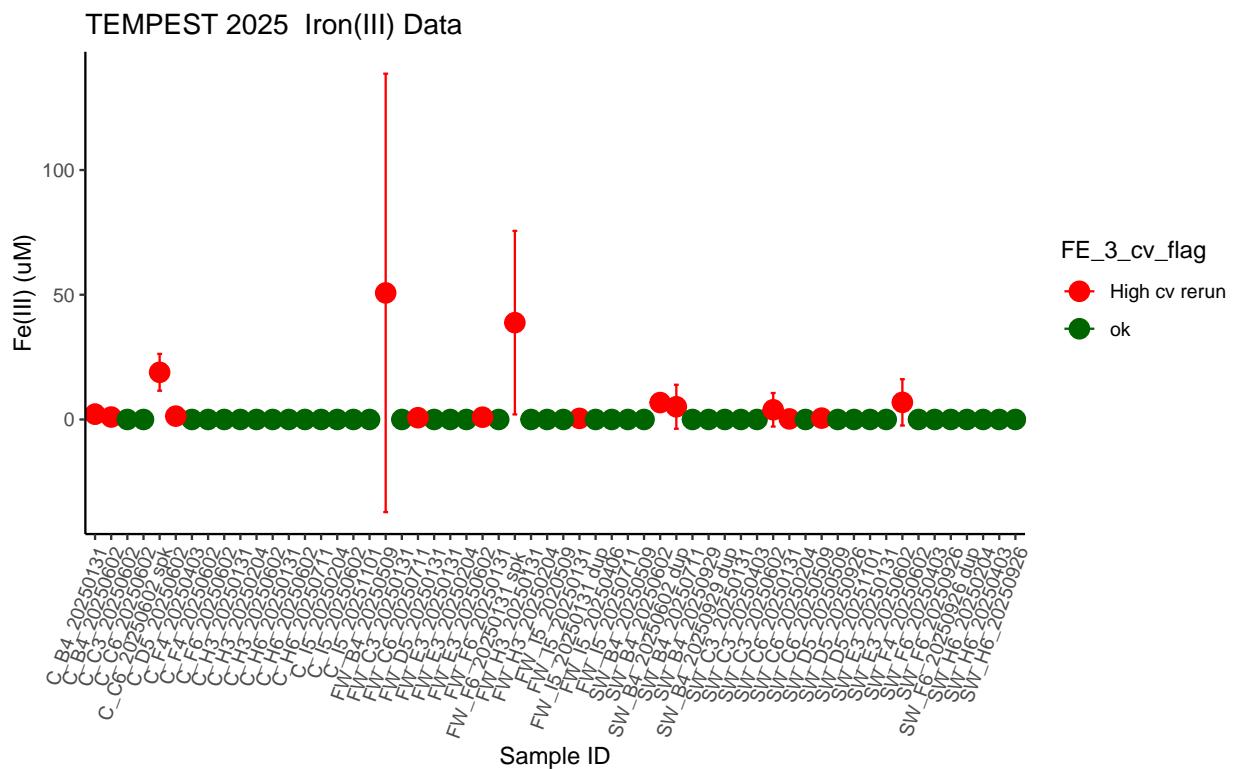
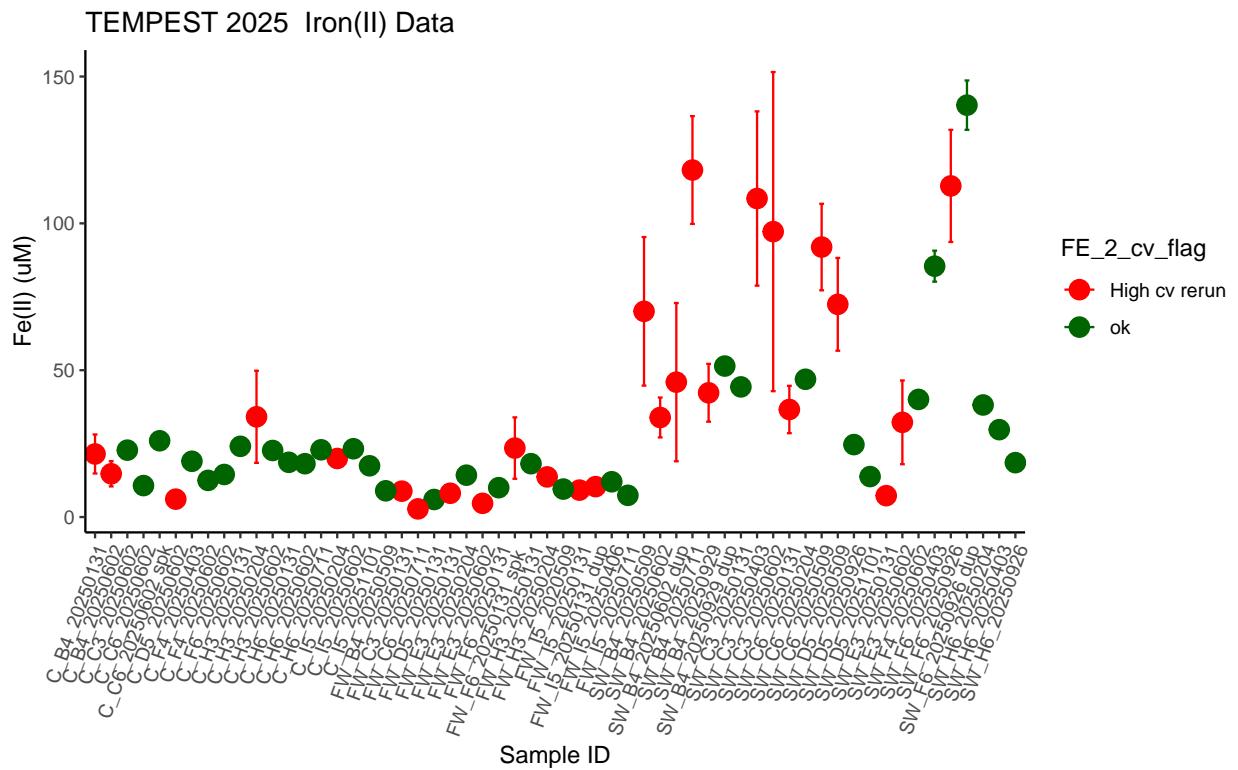
Check Standards



#No Matrix Checks We do not use matrix checks for the Fe samples because our matrix checks are not made with Trace metal grade reagents. If we want to do this in the future, we need to use trace metal grade sodium chloride and sodium bicarbonate for making the matrix checks

Subset Data and Calculate Concentrations

Calculate Averages across wells, std. dev, and cv.



Remove Bad Reps

Flagged data

Table 3: High CV Samples

ID full	FE 2 mean	FE 2 cv	FE 3 mean	FE 3 cv	FE 2 cv flag	FE 3 cv flag
Plate1_1_FW_F6_202501317.452300 spk	0.000000	54.602791	63.758240	ok	High cv rerun	ok
Plate2_1_C_B4_20250602 12.305054	10.199488	0.000000	0.000000	High cv rerun	ok	ok
Plate2_1_C_C6_20250602 25.971879 spk	8.313892	22.359023	27.444720	ok	High cv rerun	ok
Plate2_1_C_D5_20250602 6.980317	17.979878	0.000000	0.000000	High cv rerun	ok	ok
Plate2_1_FW_C6_202507113.075510	8.161589	1.064411	115.544651	ok	High cv rerun	ok
Plate2_1_SW_B4_202506027.508809	10.038062	6.044241	1.382771	High cv rerun	ok	ok
Plate2_1_SW_C3_202506027.000675	31.154799	0.000000	0.000000	High cv rerun	ok	ok
Plate2_1_SW_E3_202506024.019475	3.135087	10.298916	97.778059	ok	High cv rerun	ok
Plate1_1_SW_C3_202504024.433456	12.192347	0.000000	0.000000	High cv rerun	ok	ok
Plate3_1_SW_F6_20250922.049507	11.878029	0.000000	0.000000	High cv rerun	ok	ok

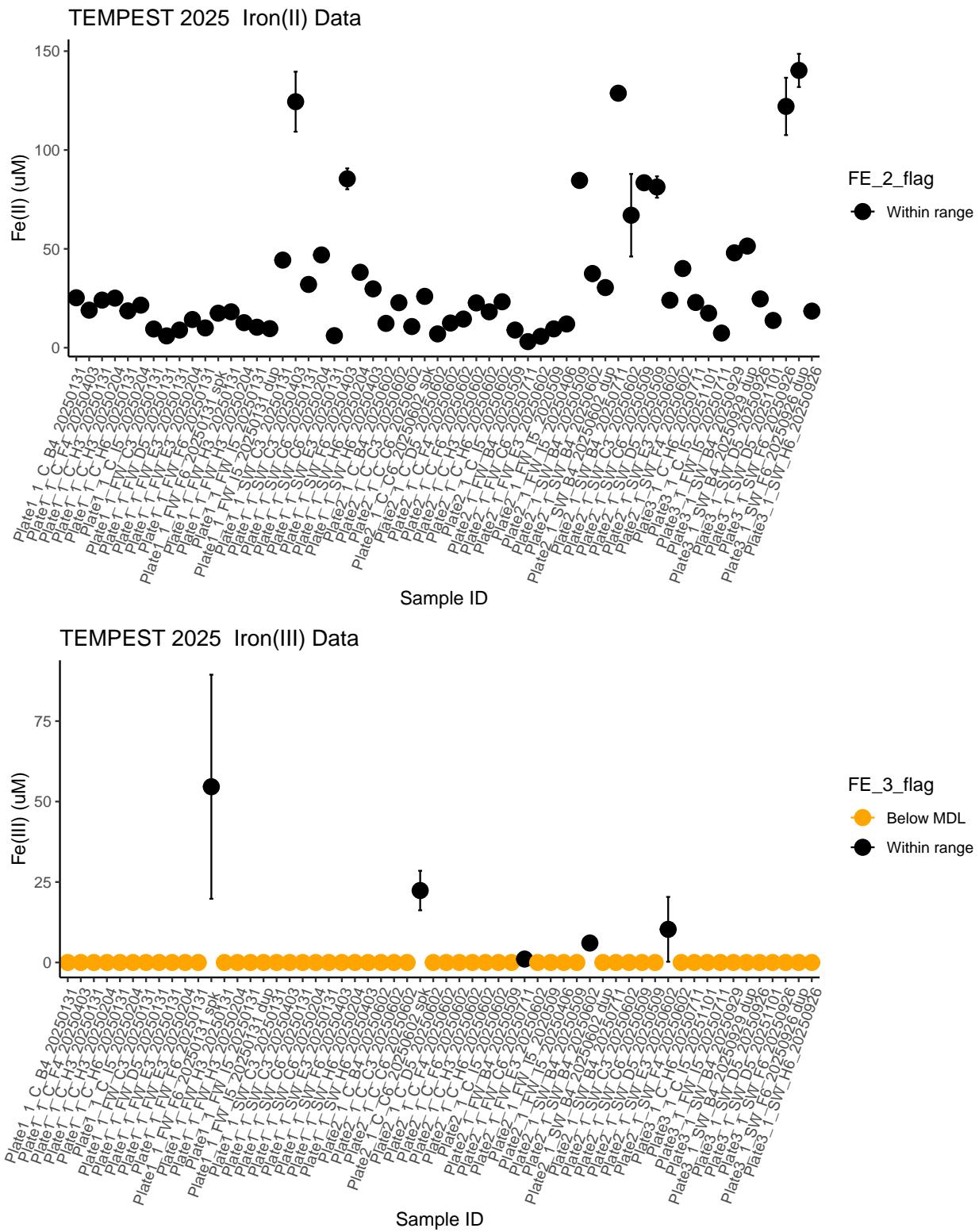
Table 4: Samples Above the Detection Limit that should be rerun at a higher dilution

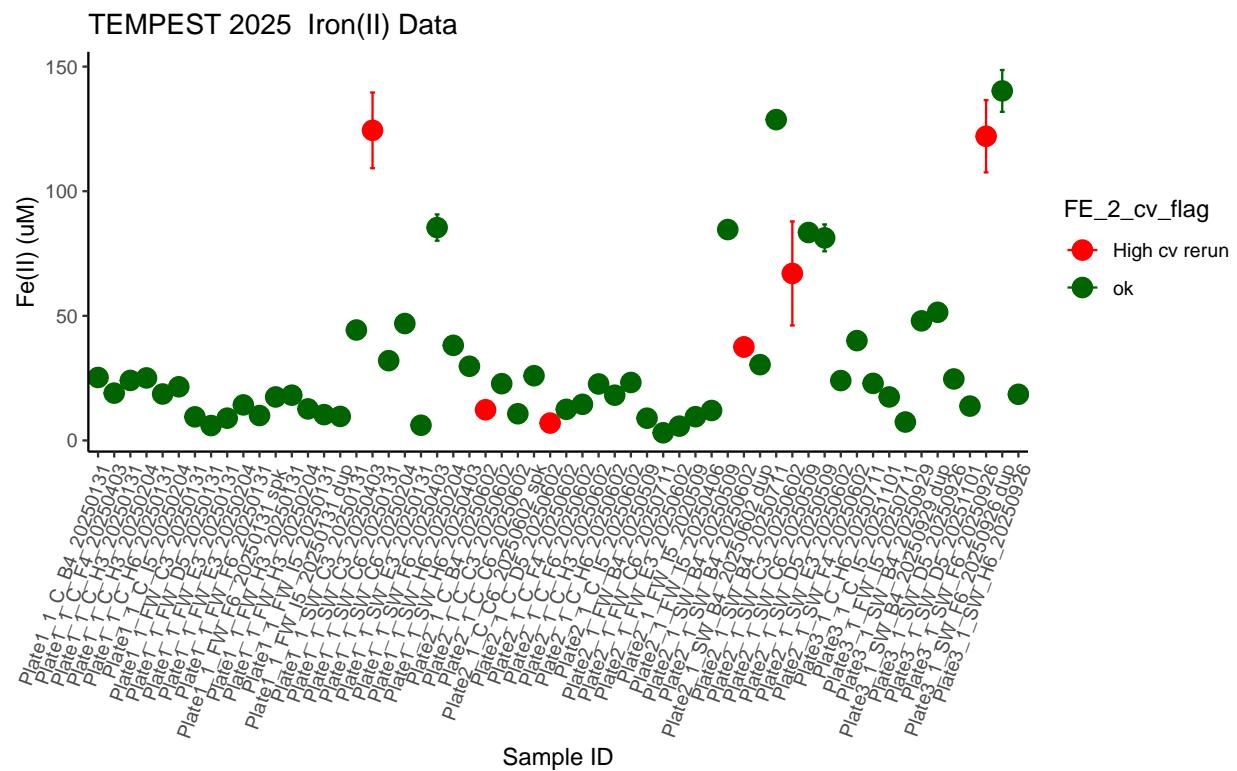
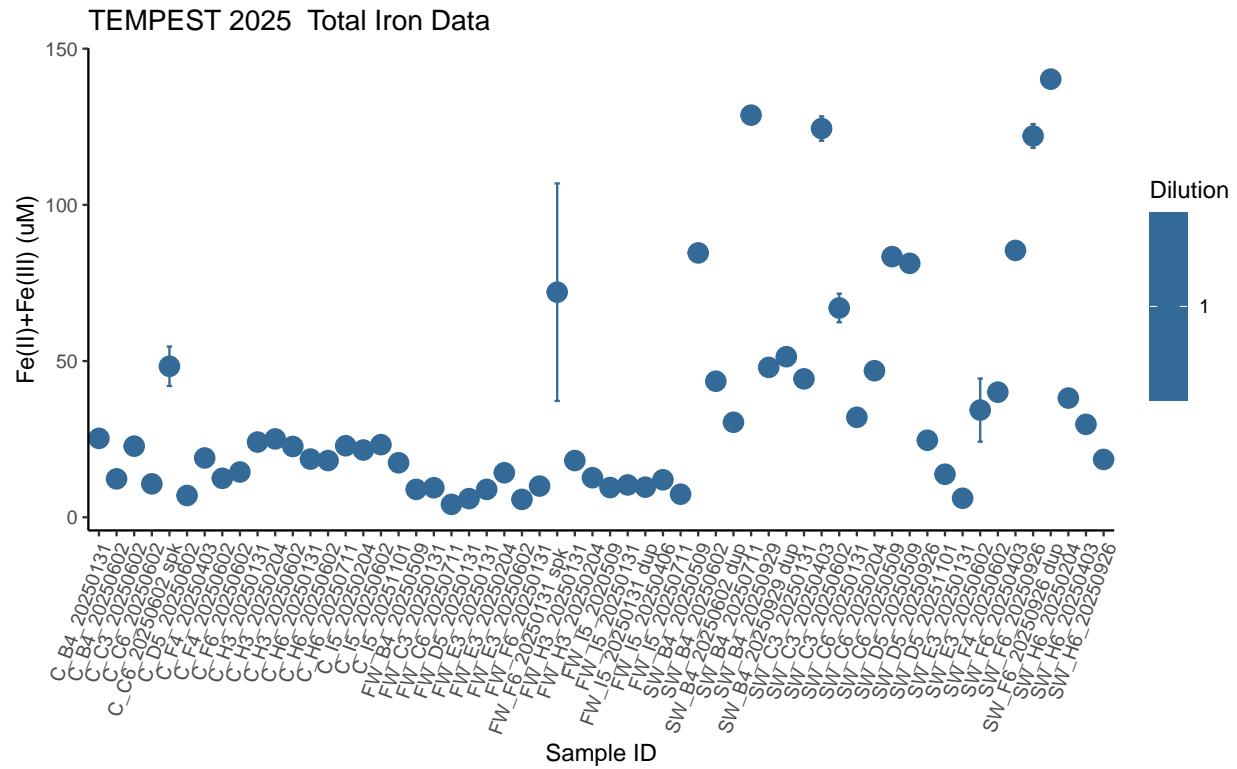
ID full	FE 2 mean	FE 3 mean	FE tot mean	FE 2 flag	FE 3 flag

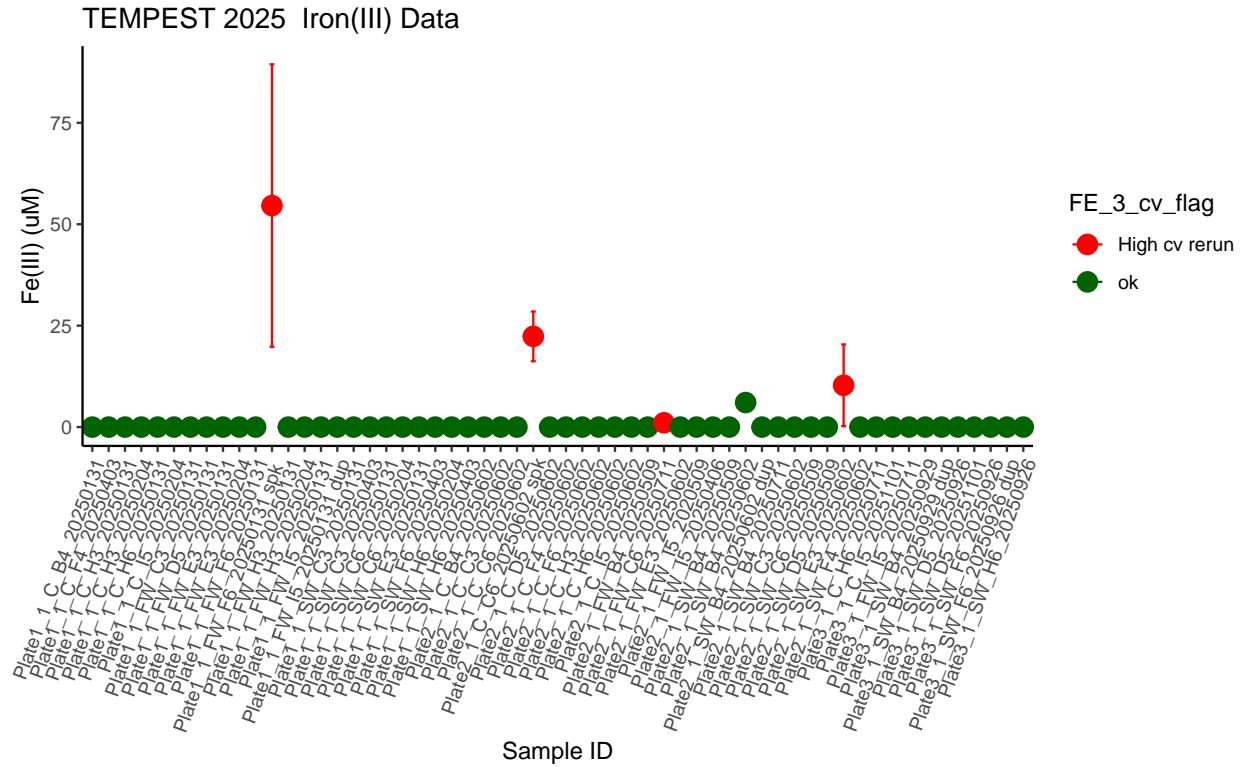
Table 5: Samples Below the Detection Limit that should be rerun at a lower dilution

ID full	FE 2 mean	FE 3 mean	FE tot mean	FE 2 flag	FE 3 flag

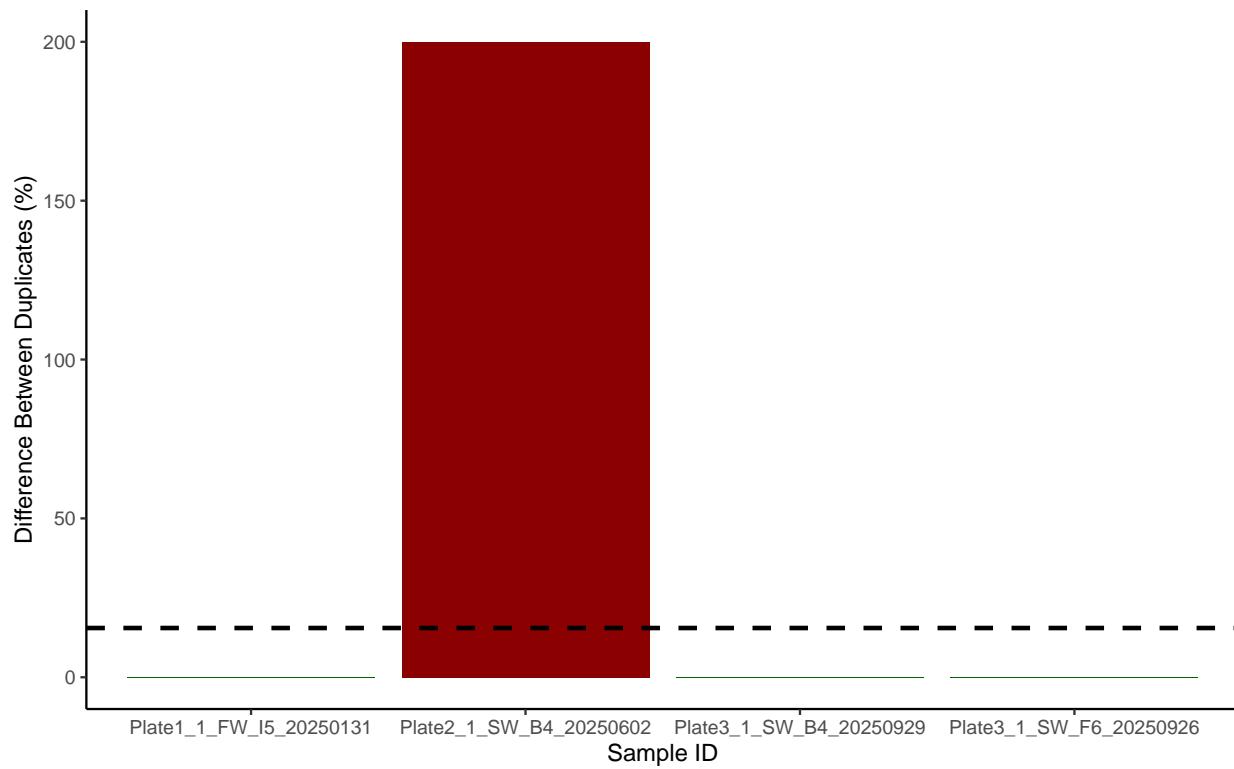
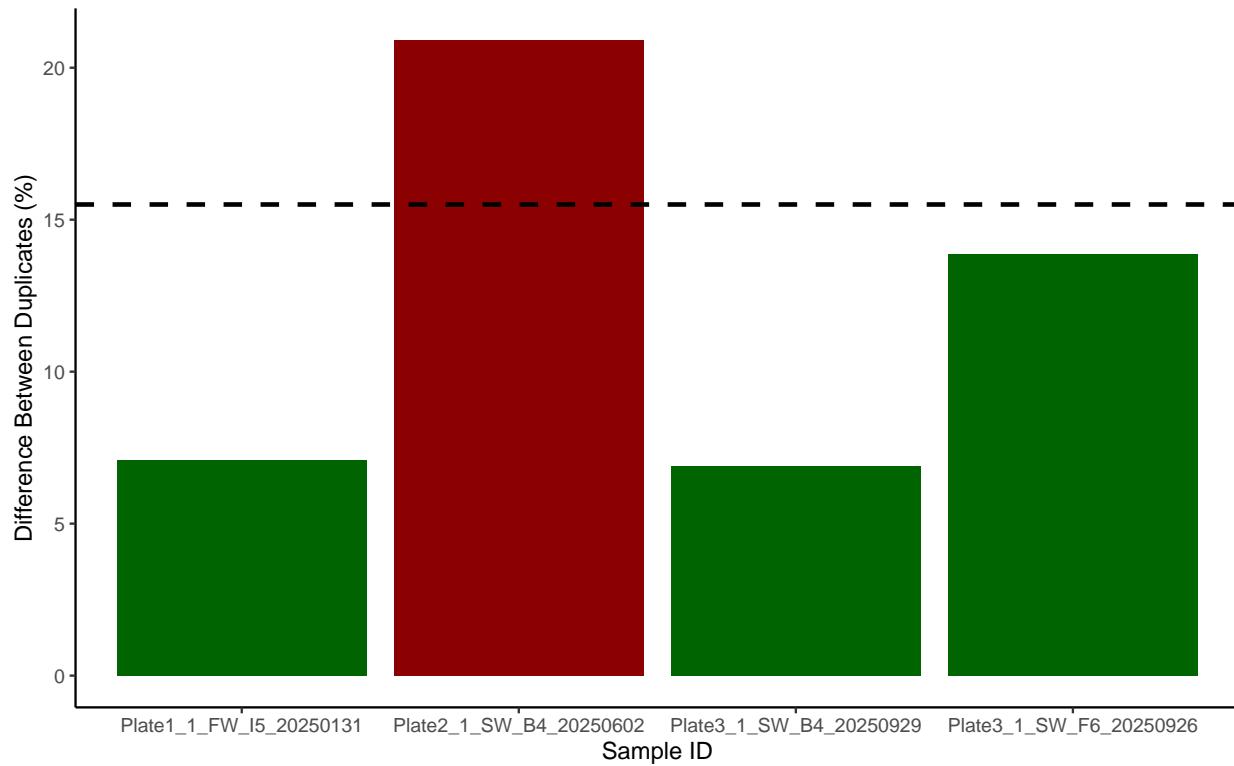
Plot data after bad reps were removed

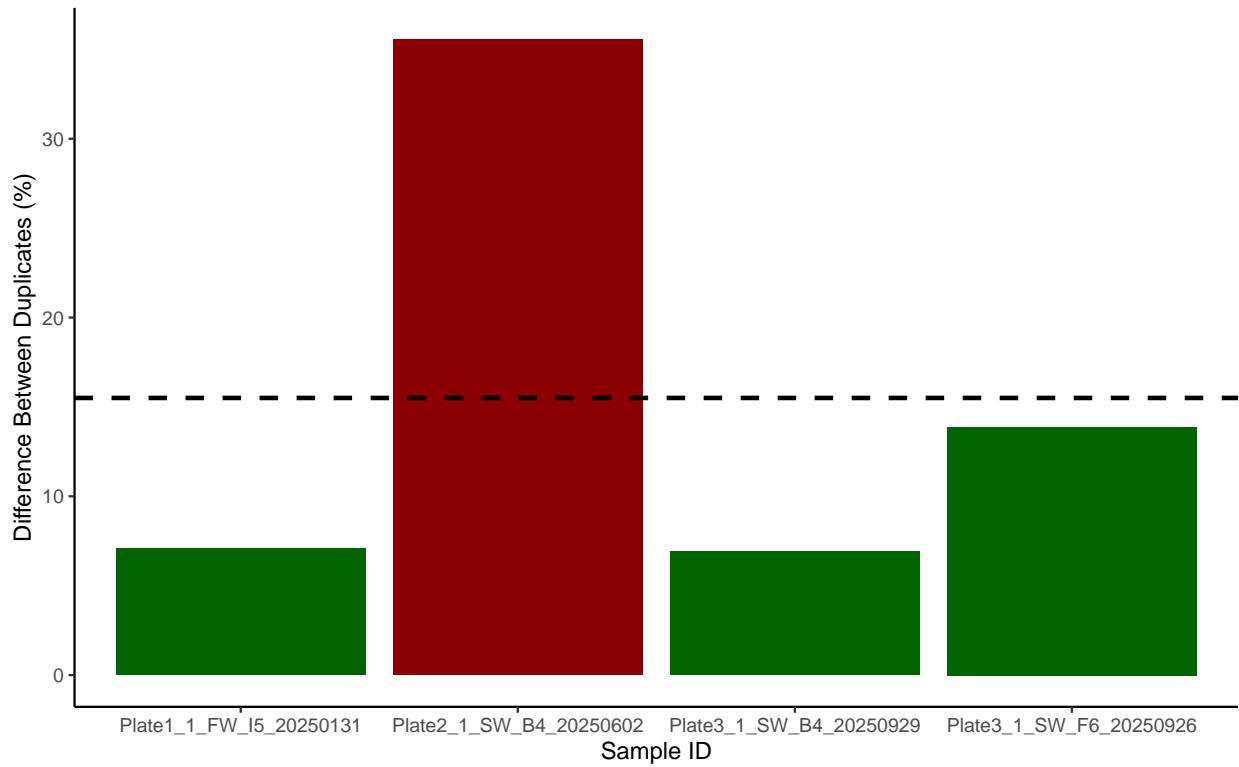






Check Dups for QAQC

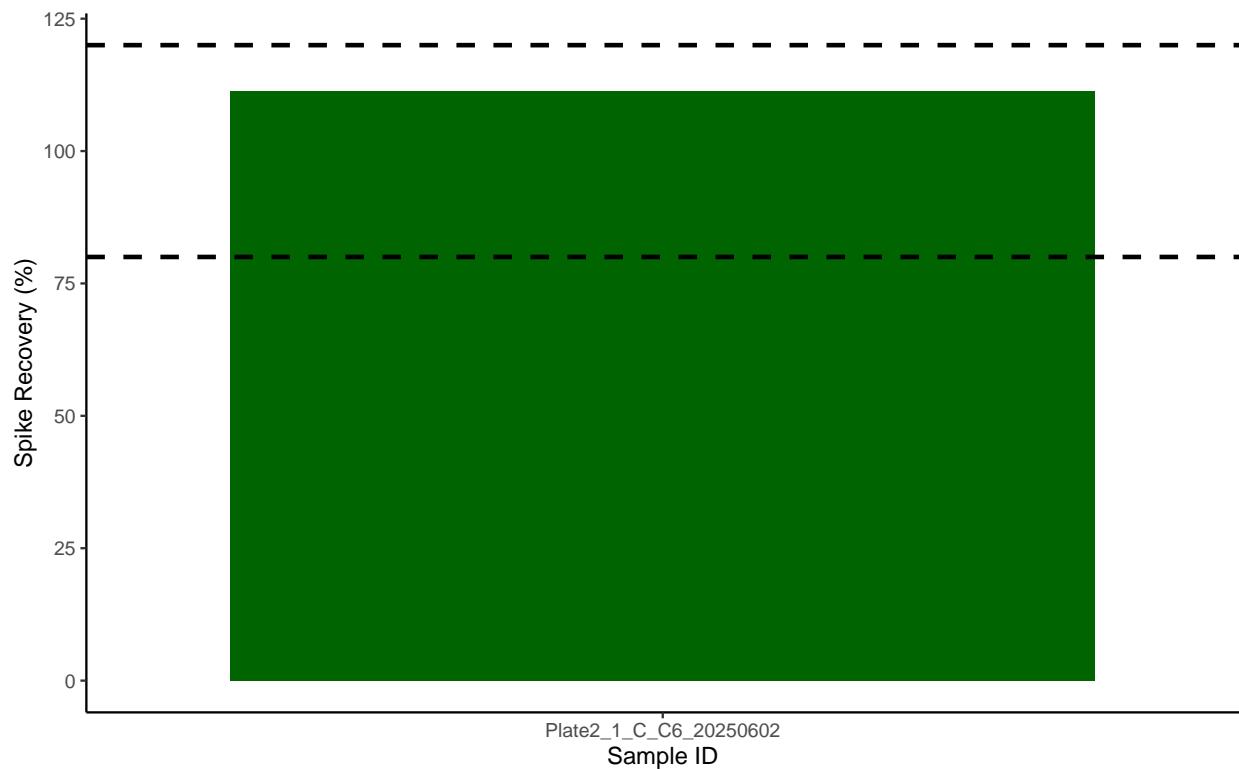




```
## [1] ">60% of Fe 2 Duplicates are within <10%"
```

```
## [1] ">60% of Fe 3 Duplicates are within <10%"
```

Check the spks for QAQC



```
## [1] ">60% of Spikes are within range"
```

Export full data then just final data