FeCode_updated2025_20260219

2026-02-24

Things that need to be changed

```
Date_Run = "20260219"
plates<- c("Plate1", "Plate2", "Plate3")
Std_plates<- c("STD")
Run_by = "Zoe Read"#Instrument user
Script_run_by ="Zoe Read"#Code user
Project = "TEMPEST"
Experiment="2025"
Run_notes="Standard curve was better on 20260218, so used that curve instead of the one ran on 20260219

#Stds that should be excluded
stds_to_remove<-c("6 uM Fe_2 F", "3 uM Fe_3 G")
```
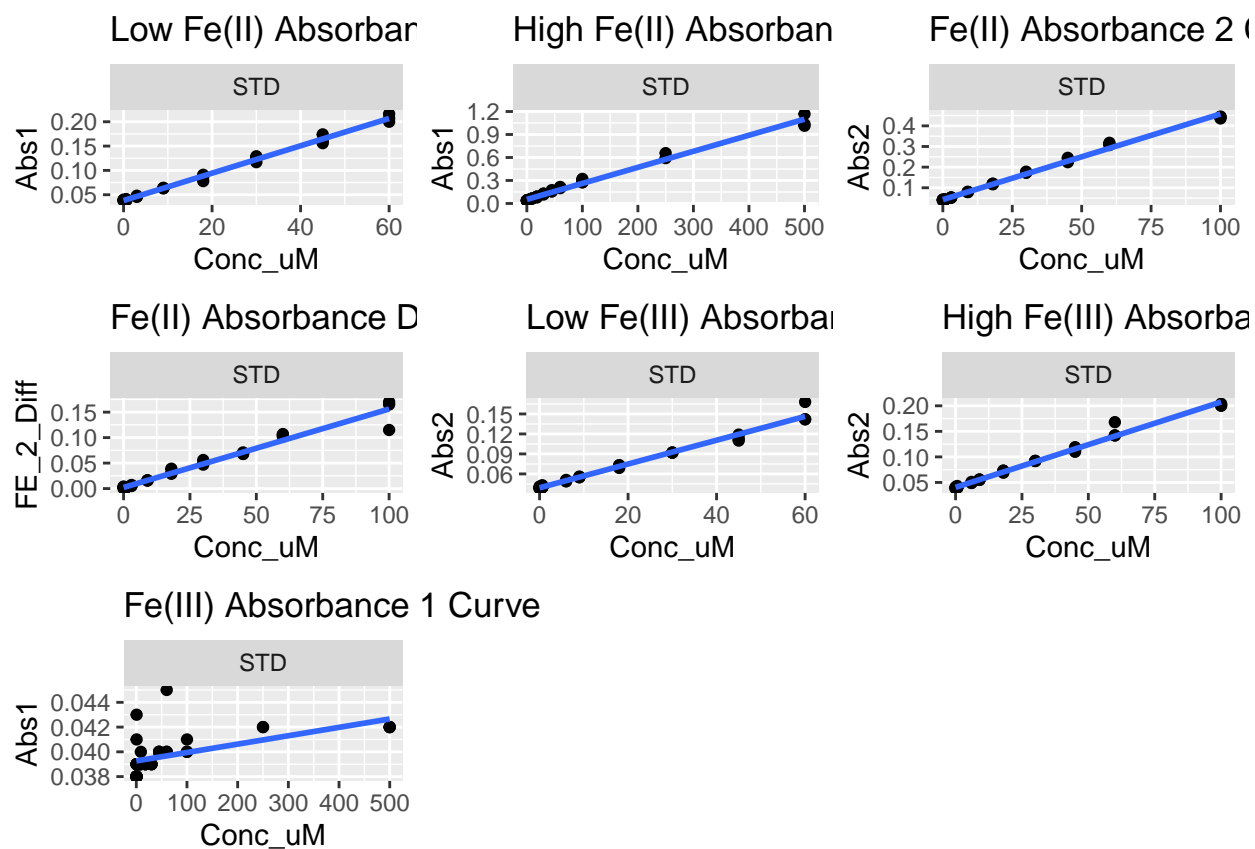
File paths

```
## [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"
```
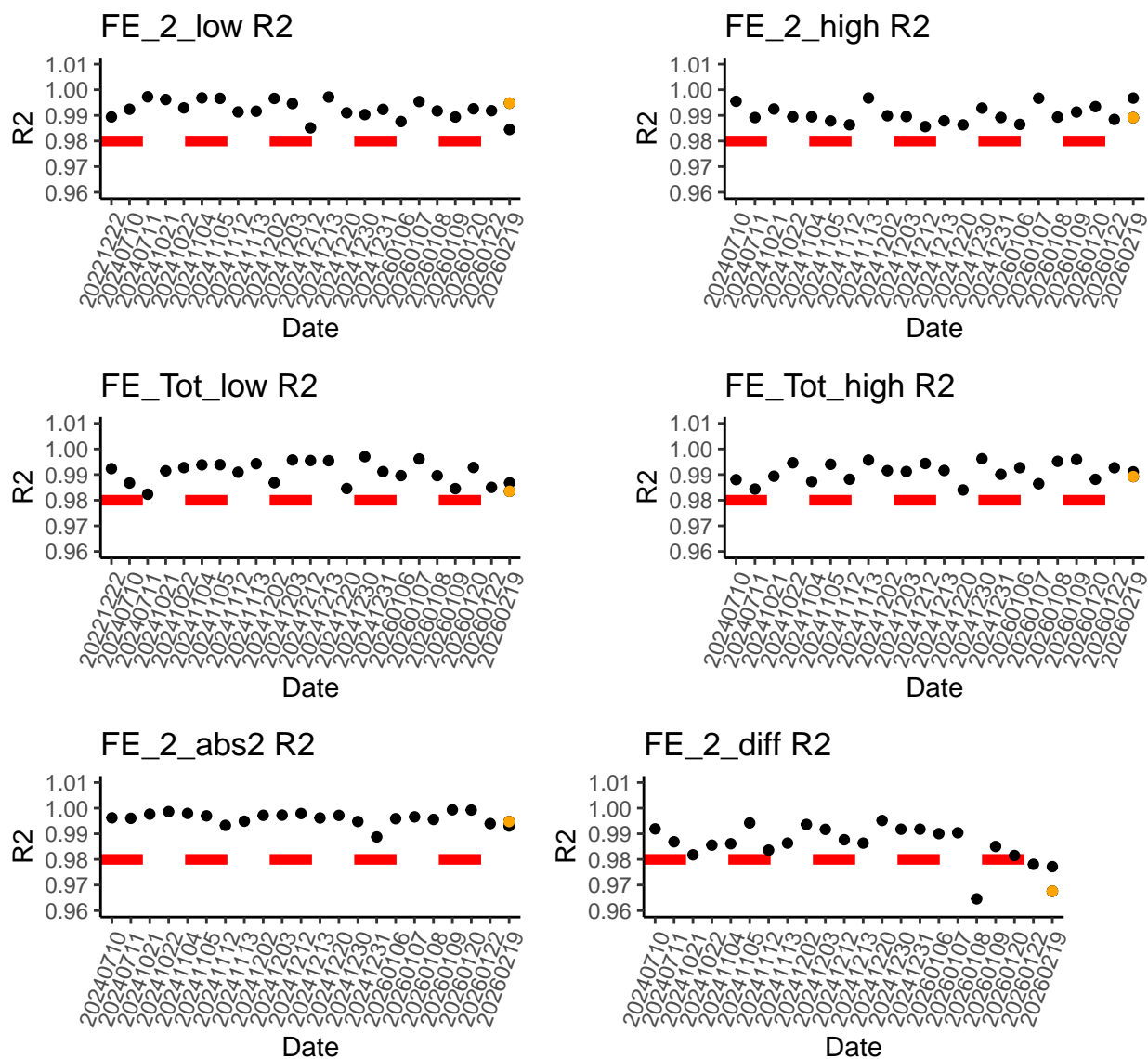
Plot standards

Table 1: Slopes

Date	Project	Curve	R2	Slope	Intercept	Top_STD
20260219	TEMPEST	FE_2_low	0.9947841	0.0028131	0.0380602	60
20260219	TEMPEST	FE_2_high	0.9891119	0.0020944	0.0525556	500
20260219	TEMPEST	FE_Tot_low	0.9834995	0.0017856	0.0391580	60
20260219	TEMPEST	FE_Tot_high	0.9892345	0.0016712	0.0403968	100
20260219	TEMPEST	FE_2_abs2	0.9947698	0.0041526	0.0424366	100
20260219	TEMPEST	FE_3_abs1	0.3265374	0.0000068	0.0392671	500
20260219	TEMPEST	FE_2_diff	0.9675970	0.0015392	0.0022041	100

Low Fe(II) Absorban

STD

High Fe(II) Absorban

STD

Fe(II) Absorbance 2 (

STD

Fe(II) Absorbance D

STD

Low Fe(III) Absorba

STD

High Fe(III) Absorba

STD

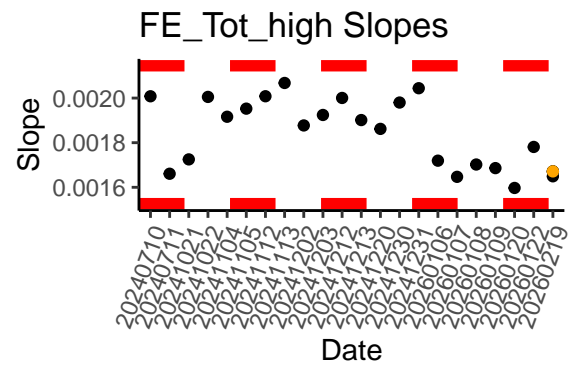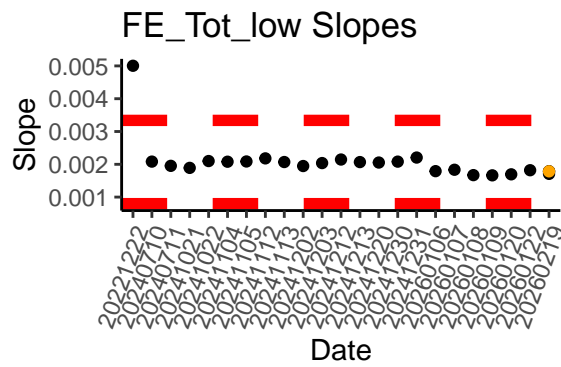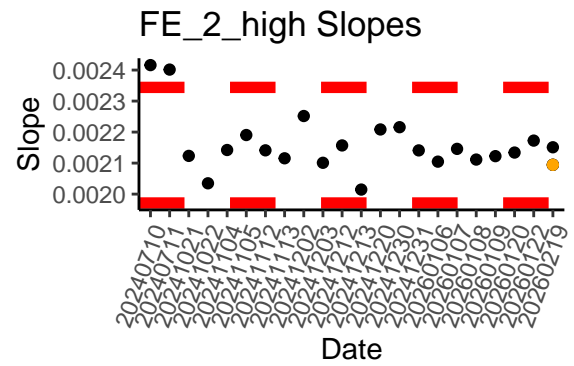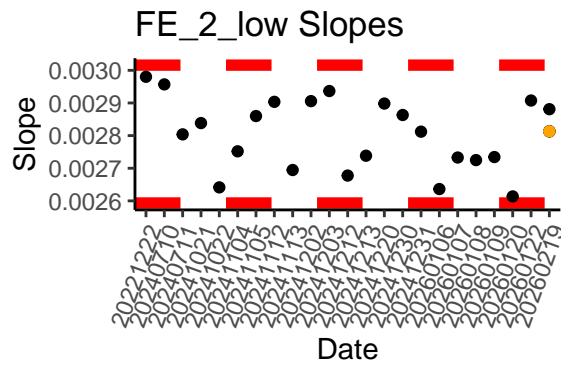## Fe(III) Absorbance 1 Curve

STD

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"
```
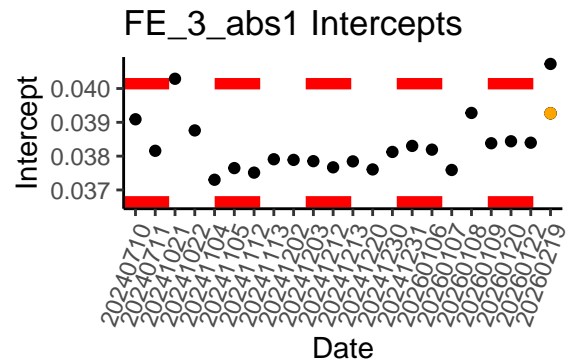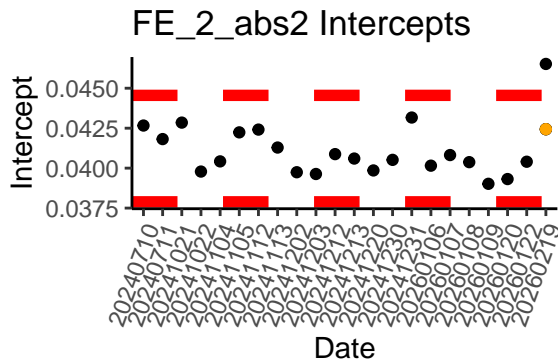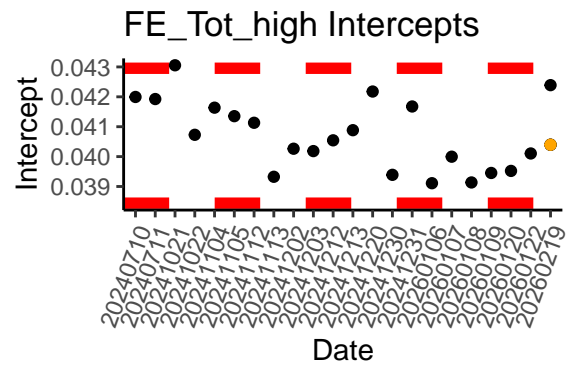
Slopes

FE_2_low Slopes

FE_2_high Slopes

FE_Tot_low Slopes

FE_Tot_high Slopes

FE_2_abs2 Slopes

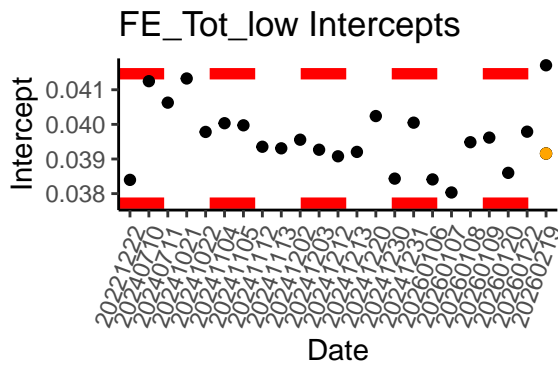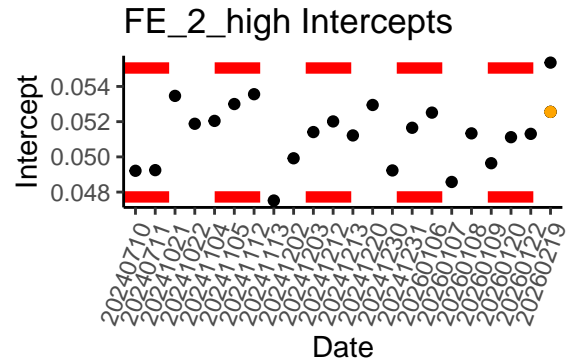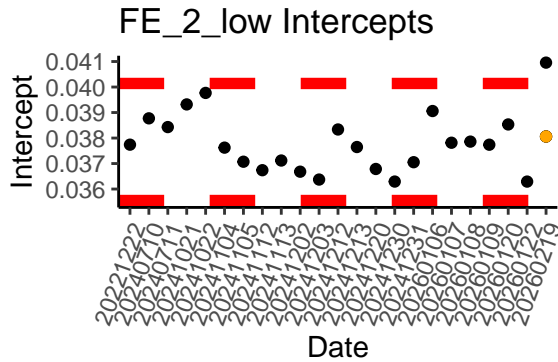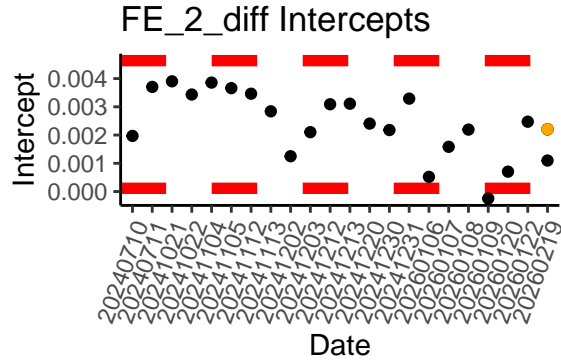
FE_3_abs1 Slopes

FE_2_diff Slopes
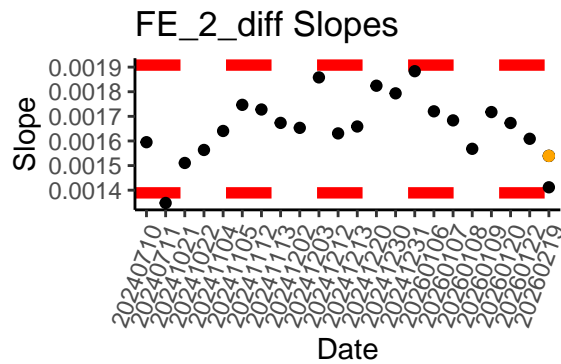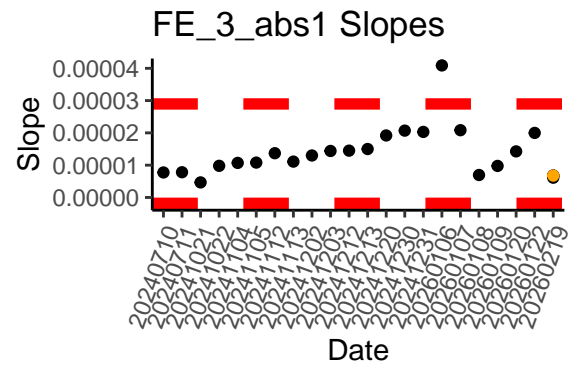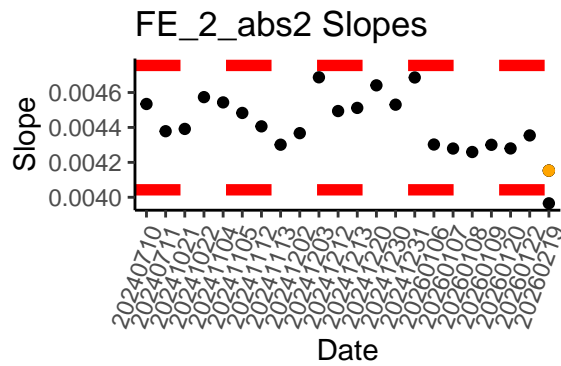

```
## [1] "FE_2_low:Std curve slope is with 2 sd of previous slopes"
## [1] "FE_2_high:Std curve slope is with 2 sd of previous slopes"
```

```
## [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

FE_2_low Intercepts

FE_2_high Intercepts

FE_Tot_low Intercepts

FE_Tot_high Intercepts

FE_2_abs2 Intercepts

FE_3_abs1 Intercepts

FE_2_diff 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
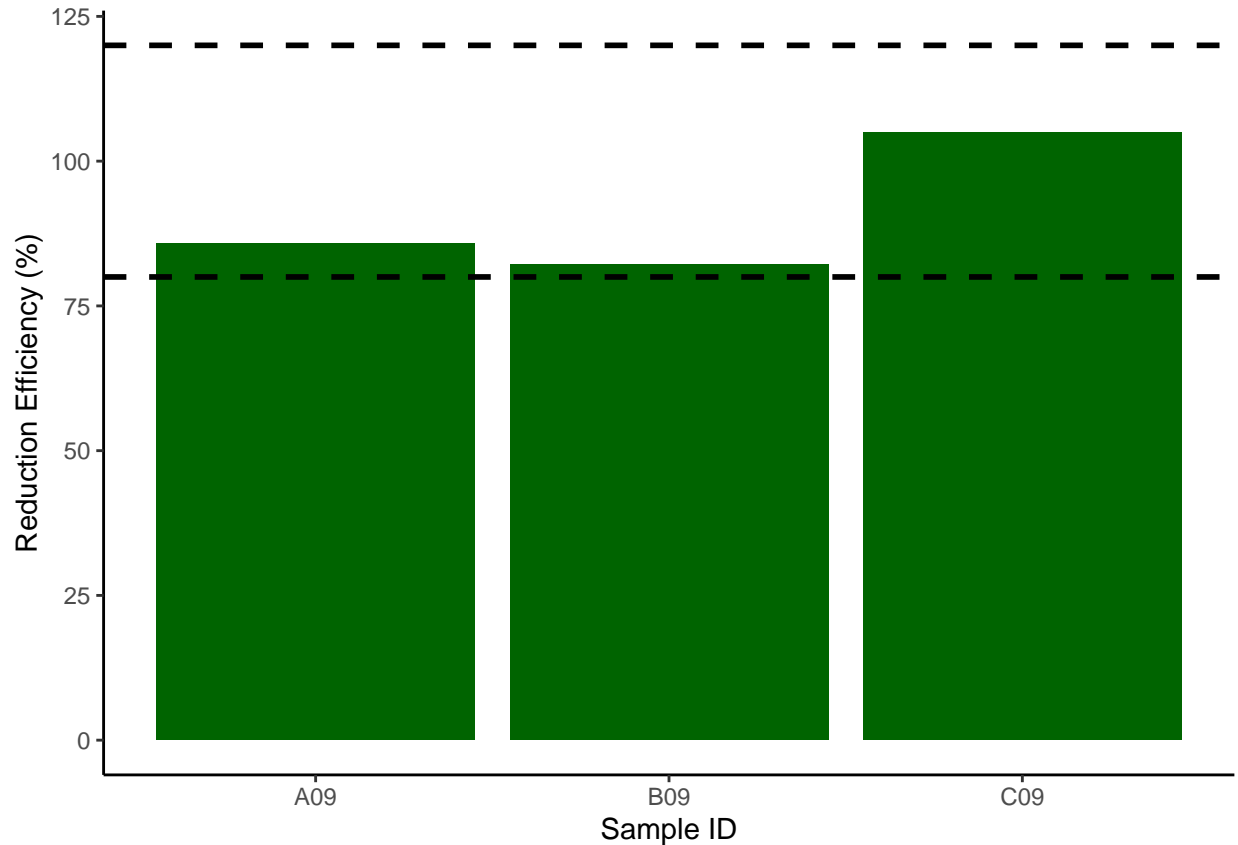
```
## [1] ">60% of Reduction Efficiencies are within range"
```

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 signficantly different from Std - REASSESS"
## [1] "Fe2 Chk Std 9 is signficantly 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 signficantly 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
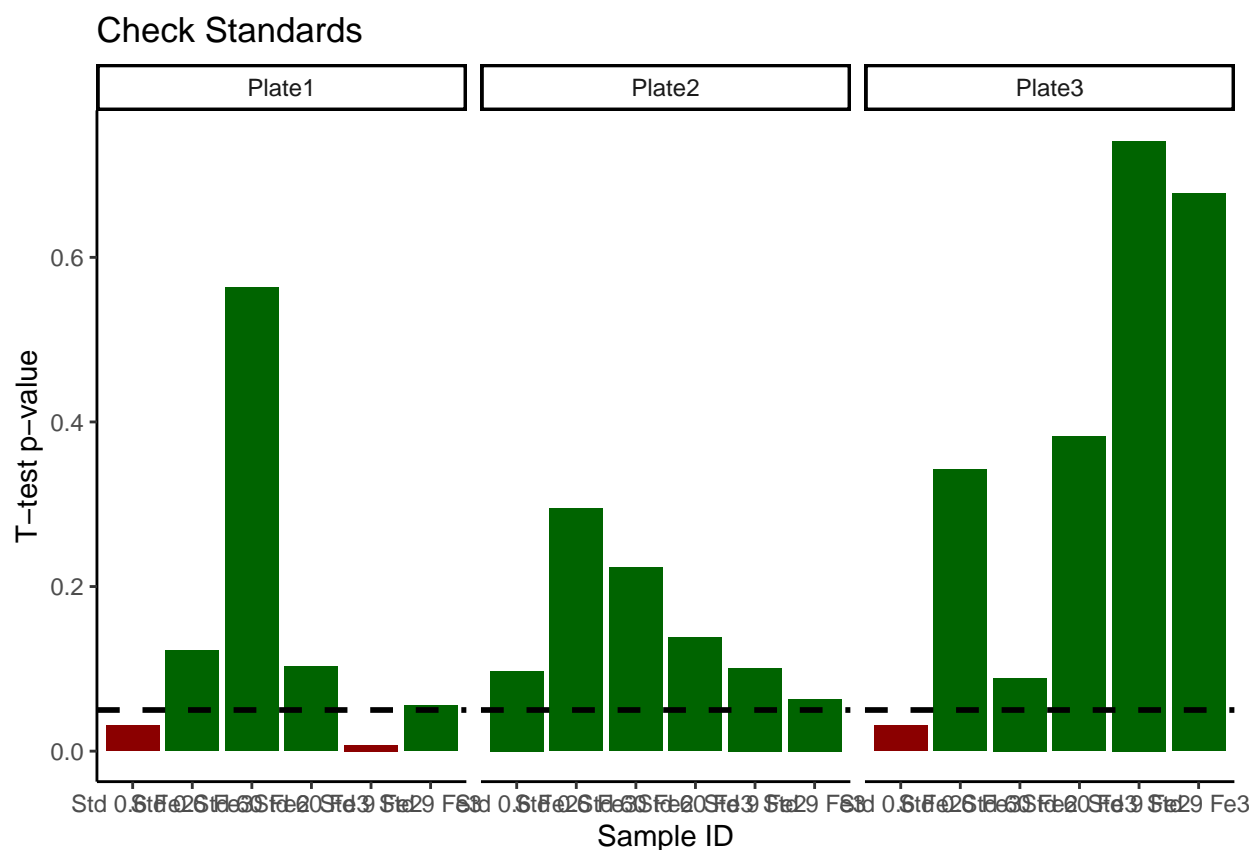
#No Matrix Checks We do not use matrix checks for the Fe samples because our matrix checks are not made with Trace metal grade reagents. If we want to do this in the future, we need to use trace metal grade sodium chloride and sodium bicarbonate for making the matrix checks

Subset Data and Calculate Concentrations

Calculate Averages across wells, std. dev, and cv.
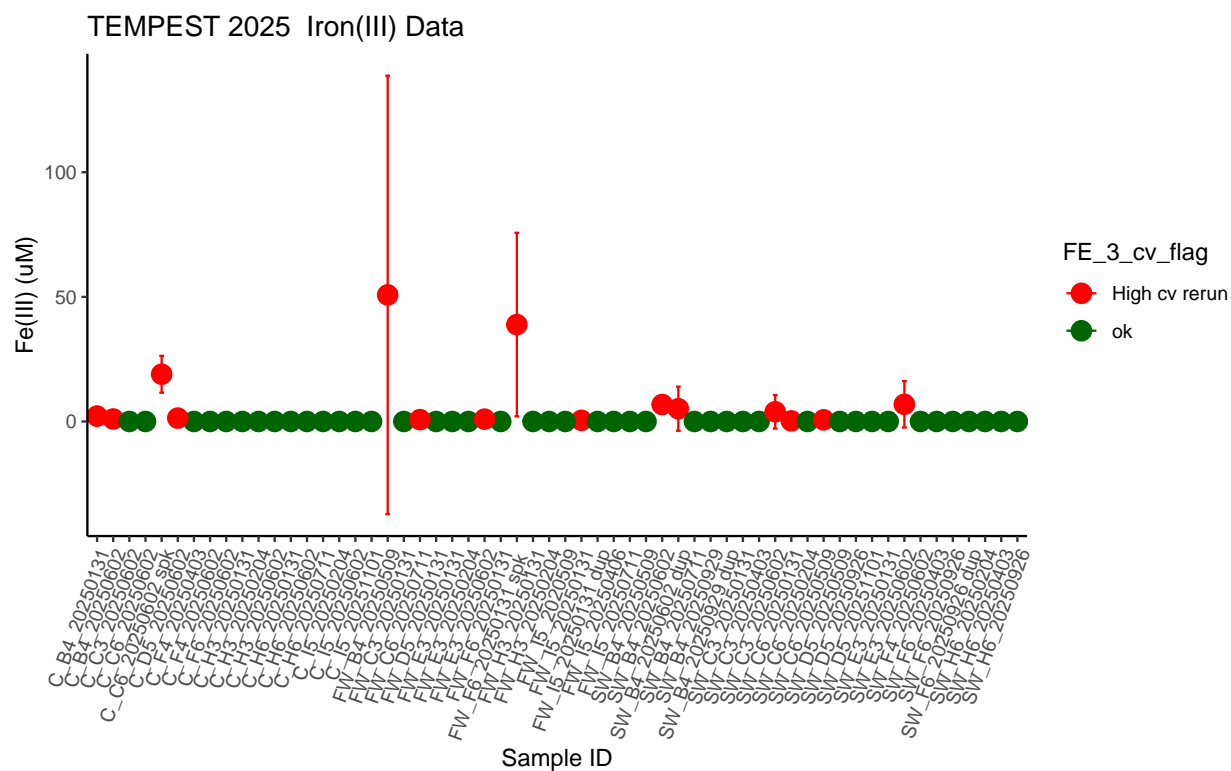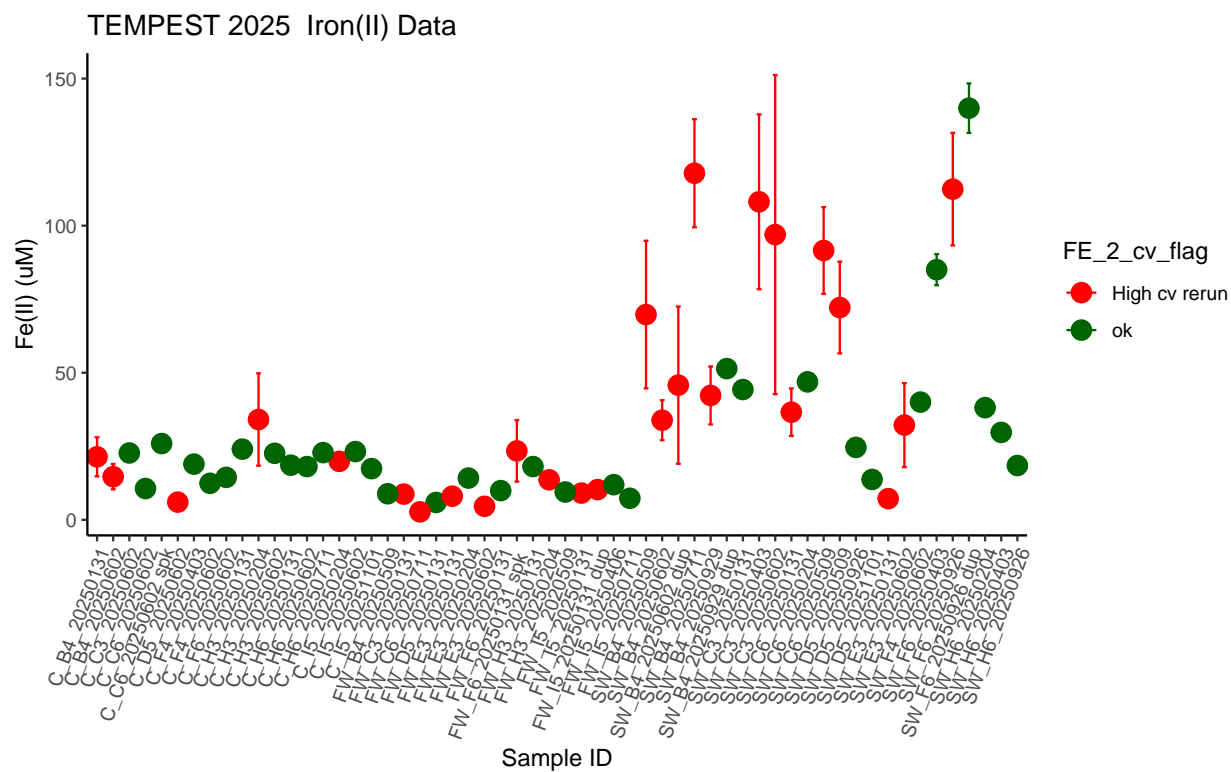
Remove Bad Reps

Flagged data

Table 3: High CV Samples

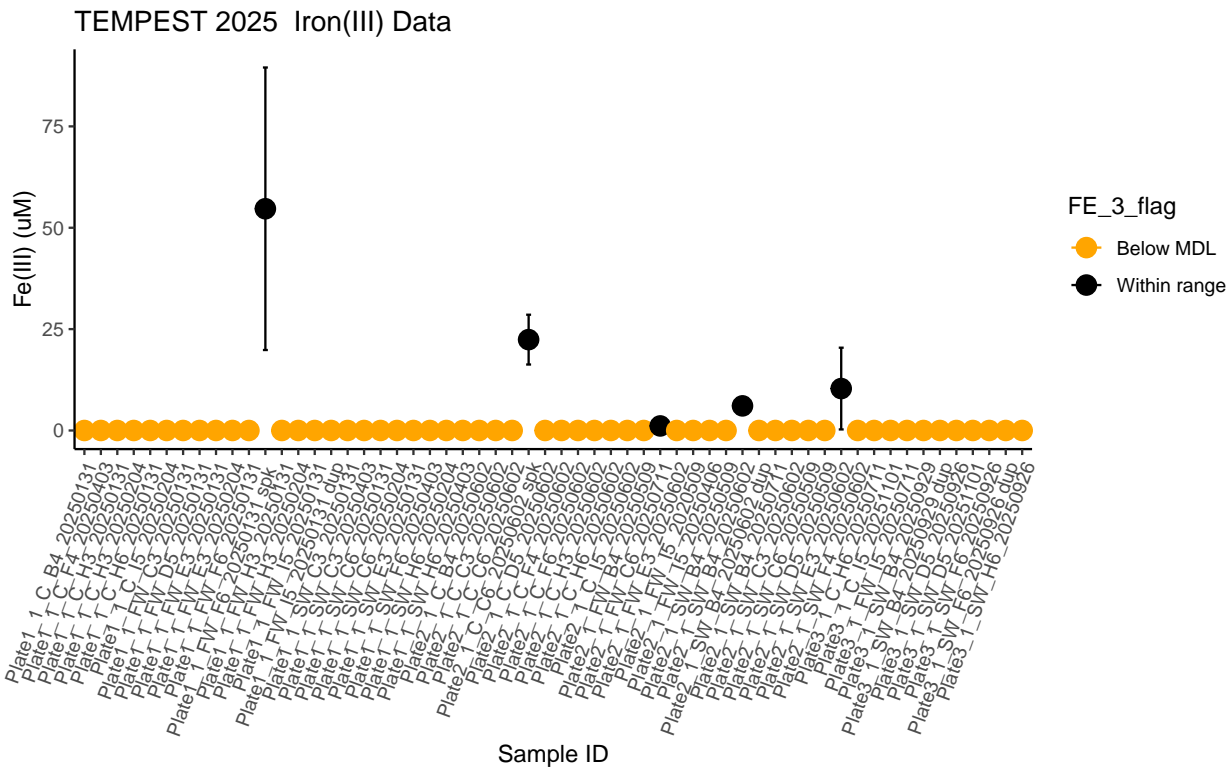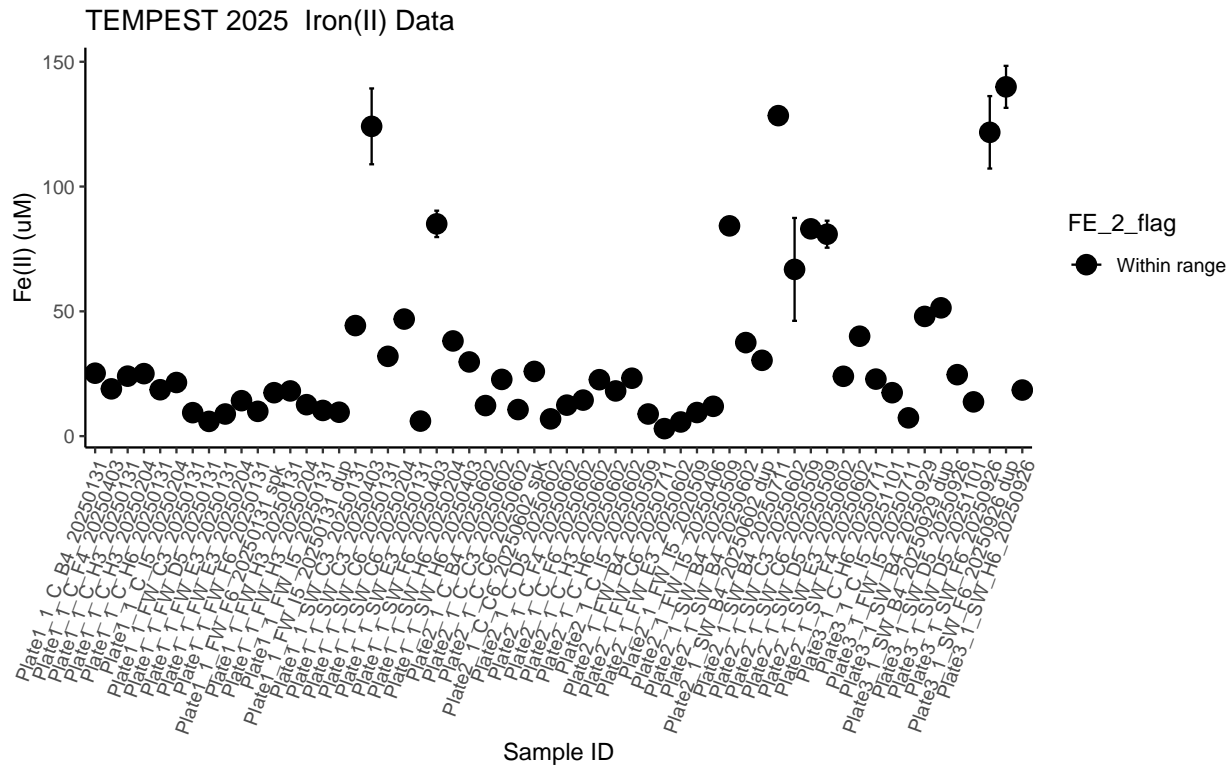| ID full	FE 2 mean	FE 2 cv	FE 3 mean	FE 3 cv	FE 2 cv flag	FE 3 cv flag
Plate1_1_FW_F6_20250131 spk	17.396826	0.000000	54.682869	63.704729	ok	High cv rerun
Plate2_1_C_B4_20250602	12.242456	10.265830	0.000000	0.000000	High cv rerun	ok
Plate2_1_C_C6_20250602 spk	25.928198	8.339426	22.410252	27.397791	ok	High cv rerun
Plate2_1_C_D5_20250602	6.910349	18.187066	0.000000	0.000000	High cv rerun	ok
Plate2_1_FW_C6_20250711	3.000137	8.378215	1.123638	109.470723	ok	High cv rerun
Plate2_1_SW_B4_20250602	7.481096	10.059389	6.070043	1.451593	High cv rerun	ok
Plate2_1_SW_C3_20250602	6.806412	30.849658	0.000000	0.000000	High cv rerun	ok
Plate2_1_SW_E3_20250602	3.973092	3.145501	10.340717	97.472339	ok	High cv rerun
Plate1_1_SW_C3_20250403	24.111815	12.241006	0.000000	0.000000	High cv rerun	ok
Plate3_1_SW_F6_20250926	21.724538	11.926364	0.000000	0.000000	High cv rerun	ok

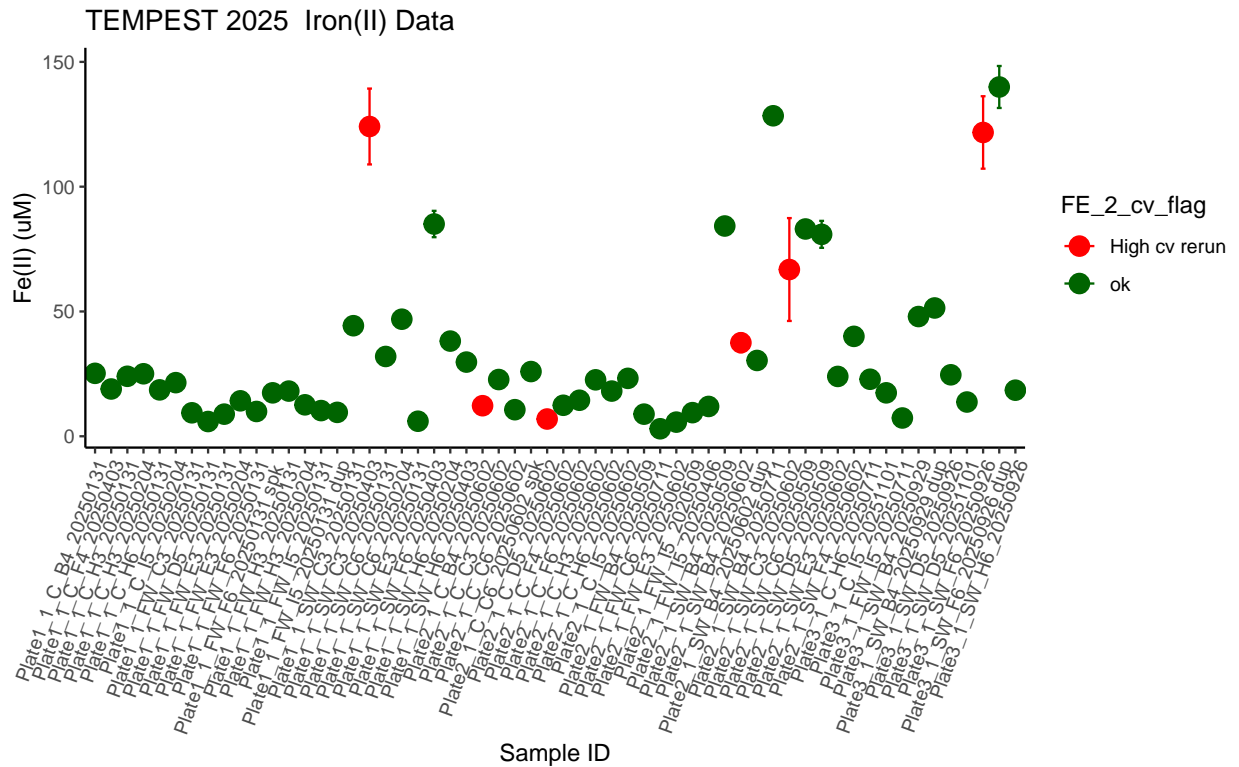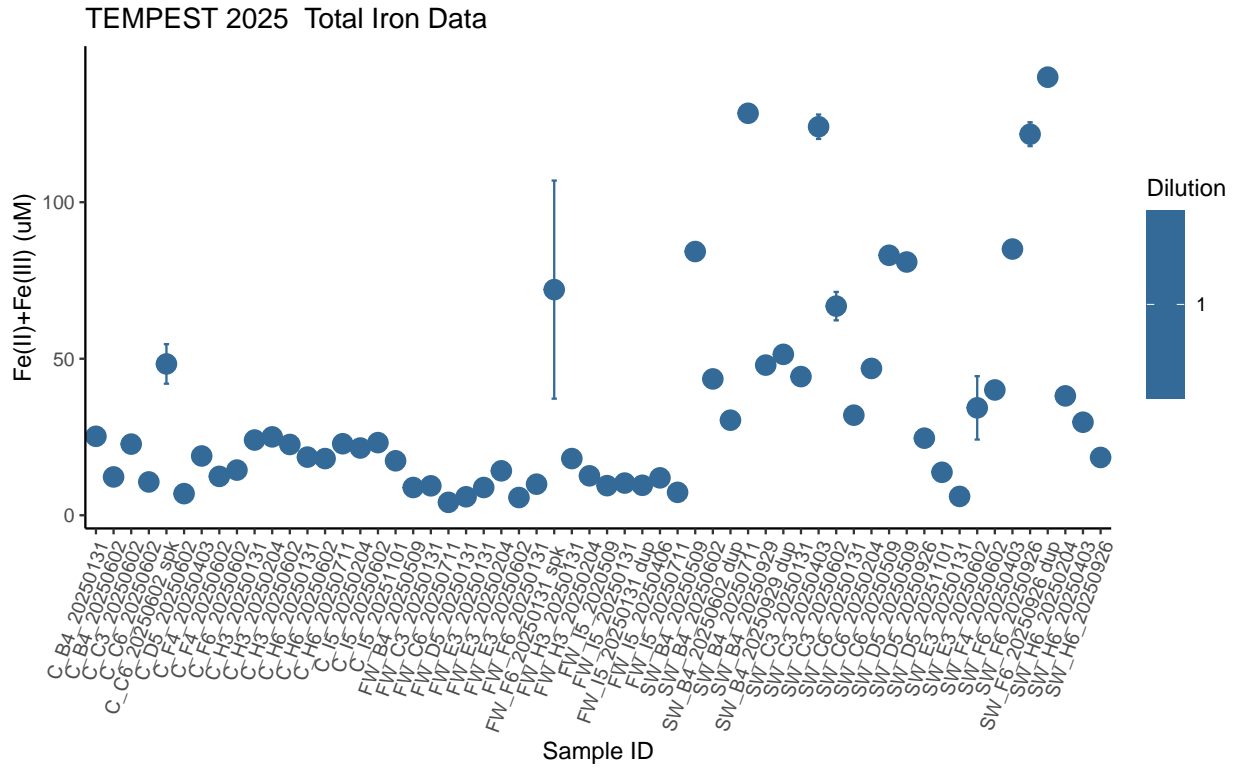Table 4: Samples Above the Detection Limit that should be rerun at a higher dilution

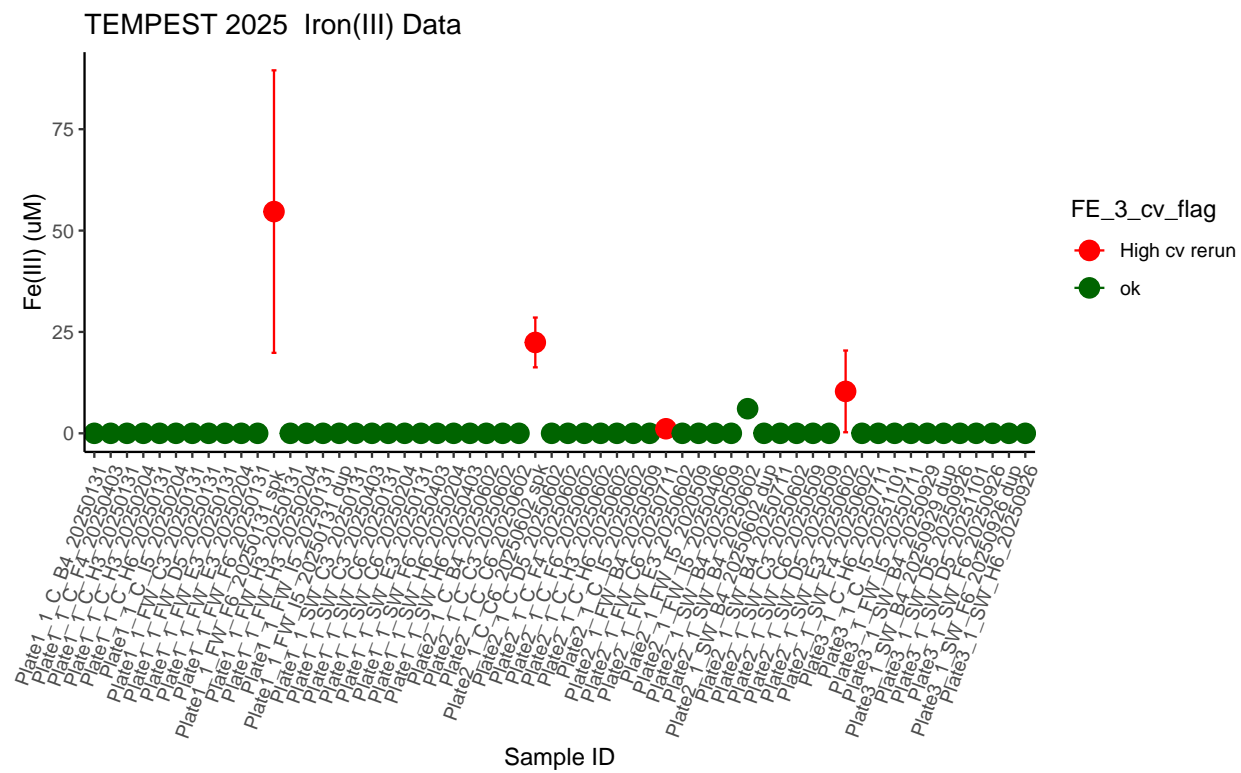| ID full	FE 2 mean	FE 3 mean	FE tot mean	FE 2 flag	FE 3 flag

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

TEMPEST 2025 Iron(II) Data

TEMPEST 2025 Iron(III) Data

TEMPEST 2025 Total Iron Data

TEMPEST 2025 Iron(II) Data

TEMPEST 2025 Iron(III) Data
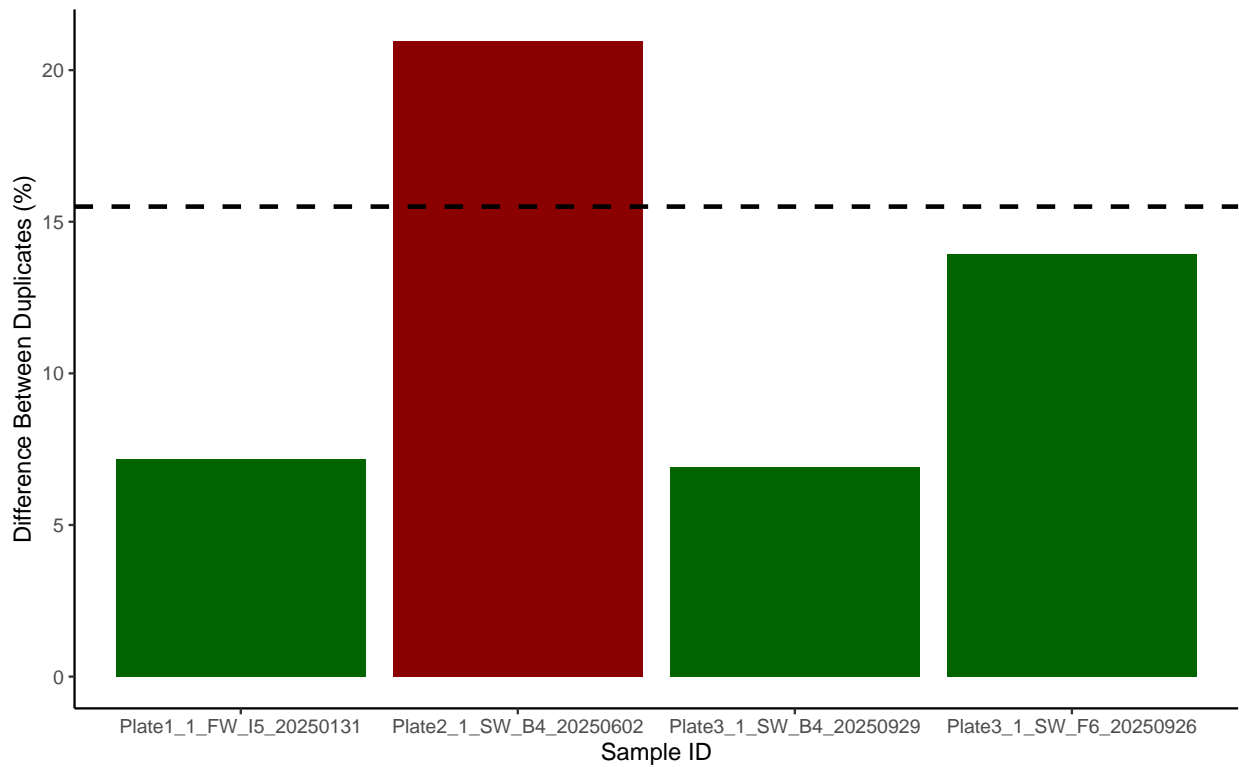
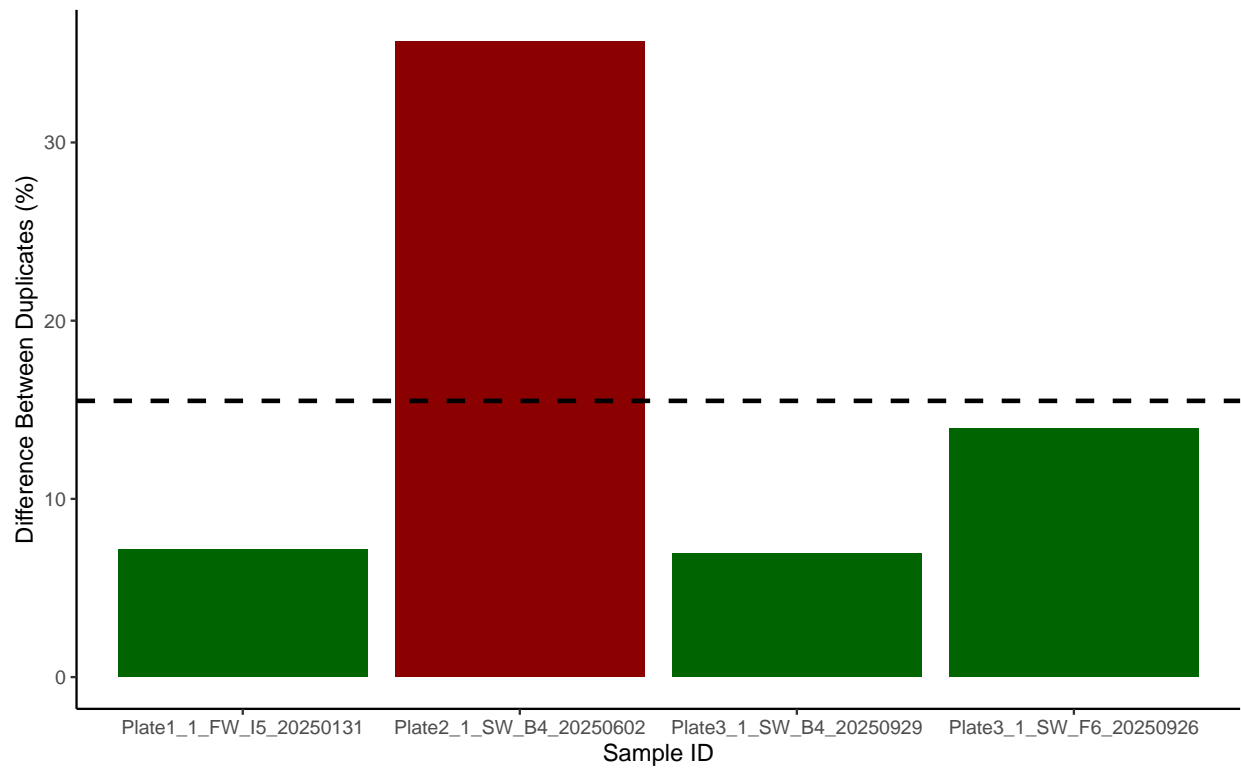# Check Dups for QAQC
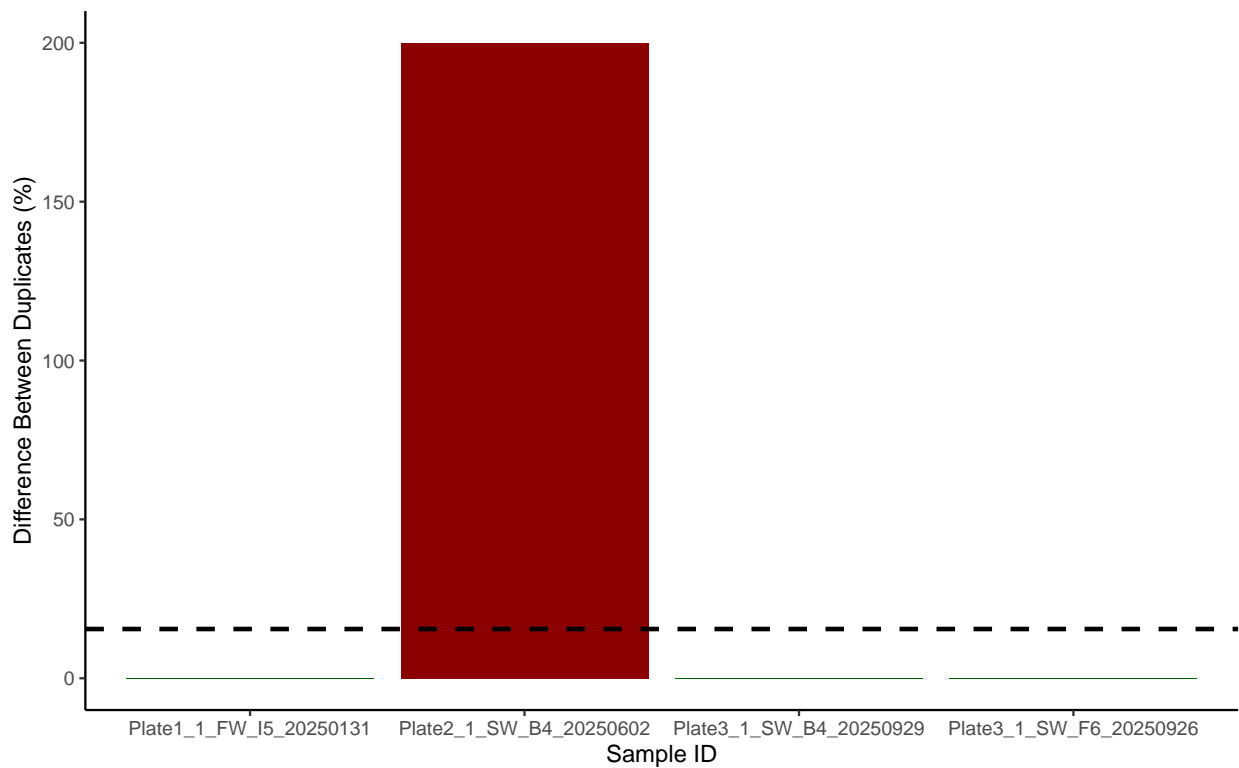
```
## [1] ">60% of Fe 2 Duplicates are within <10%"
```
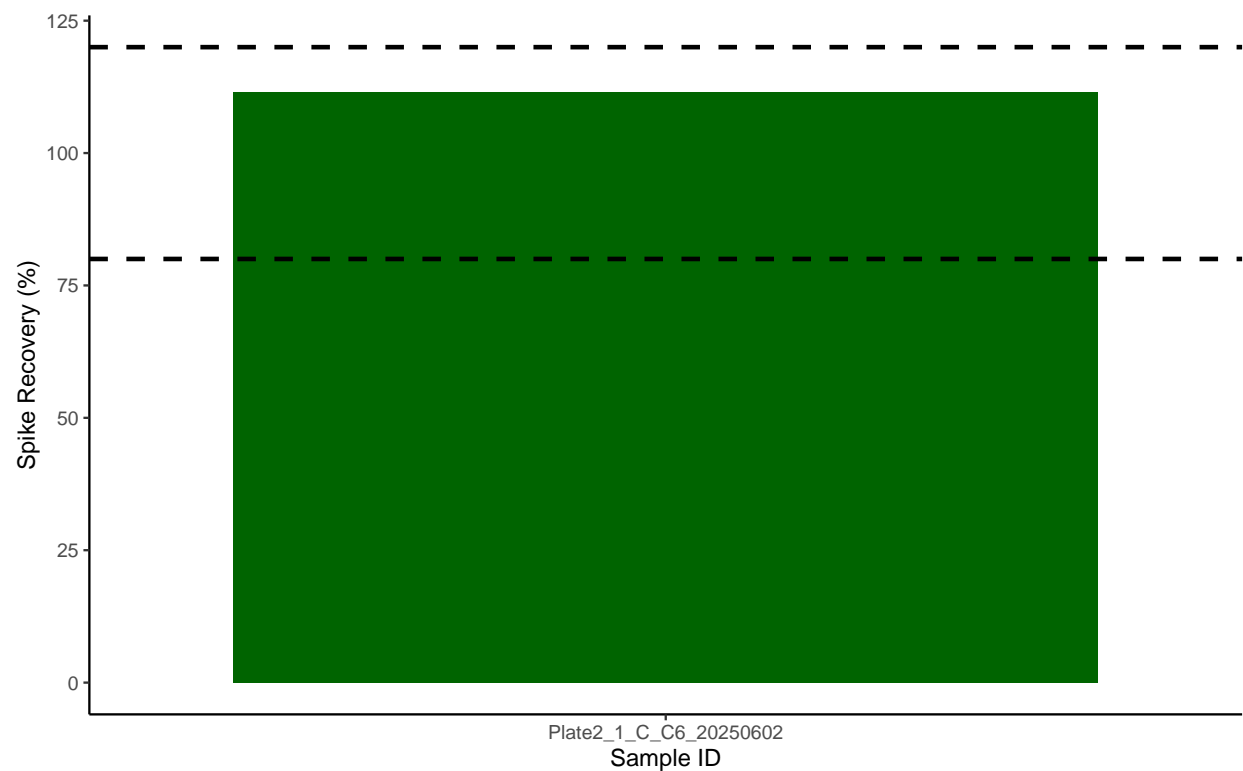
```
## [1] ">60% of Fe 3 Duplicates are within <10%"
```

Check the spks for QAQC


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

Export full data then just final data