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

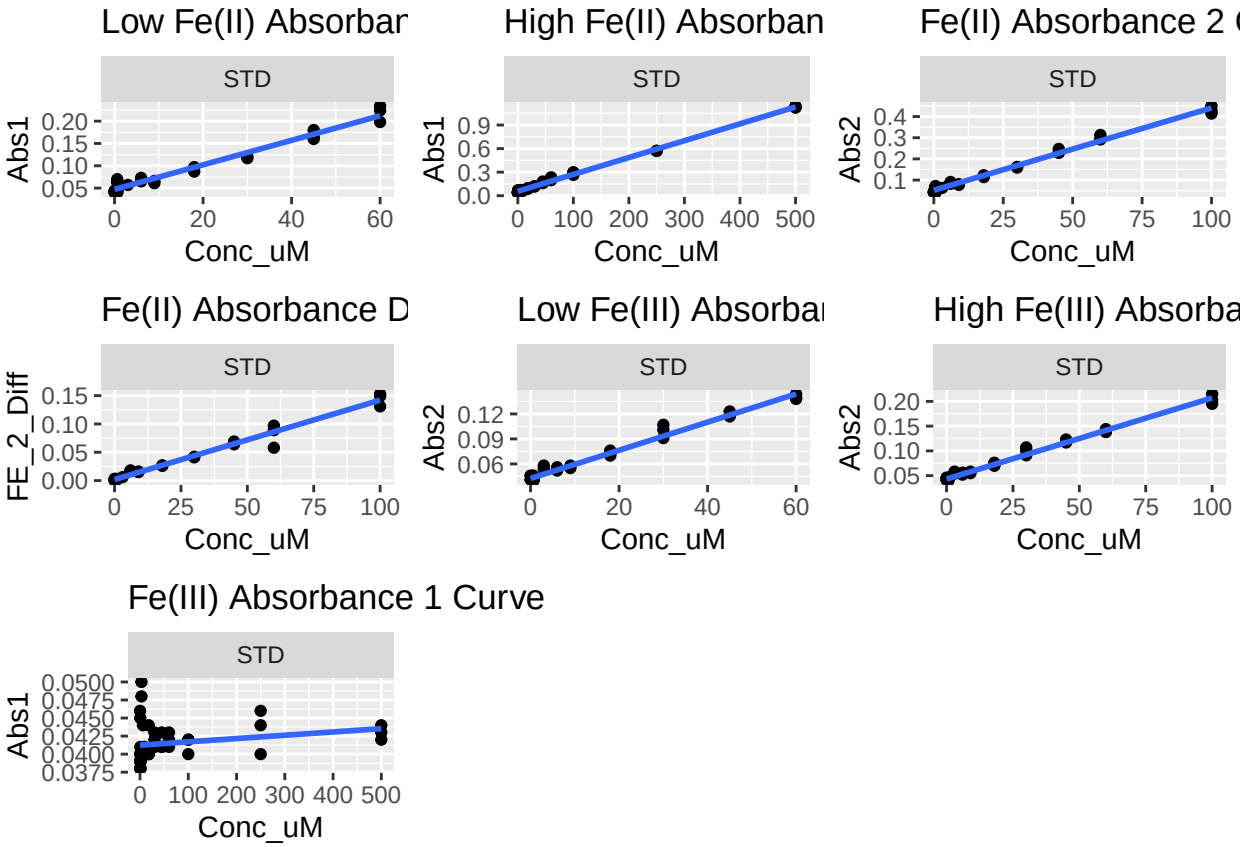
```
## [1] "Tidy Data/20260219_TEMPEST_Fe_STD.csv"
```

```
## [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

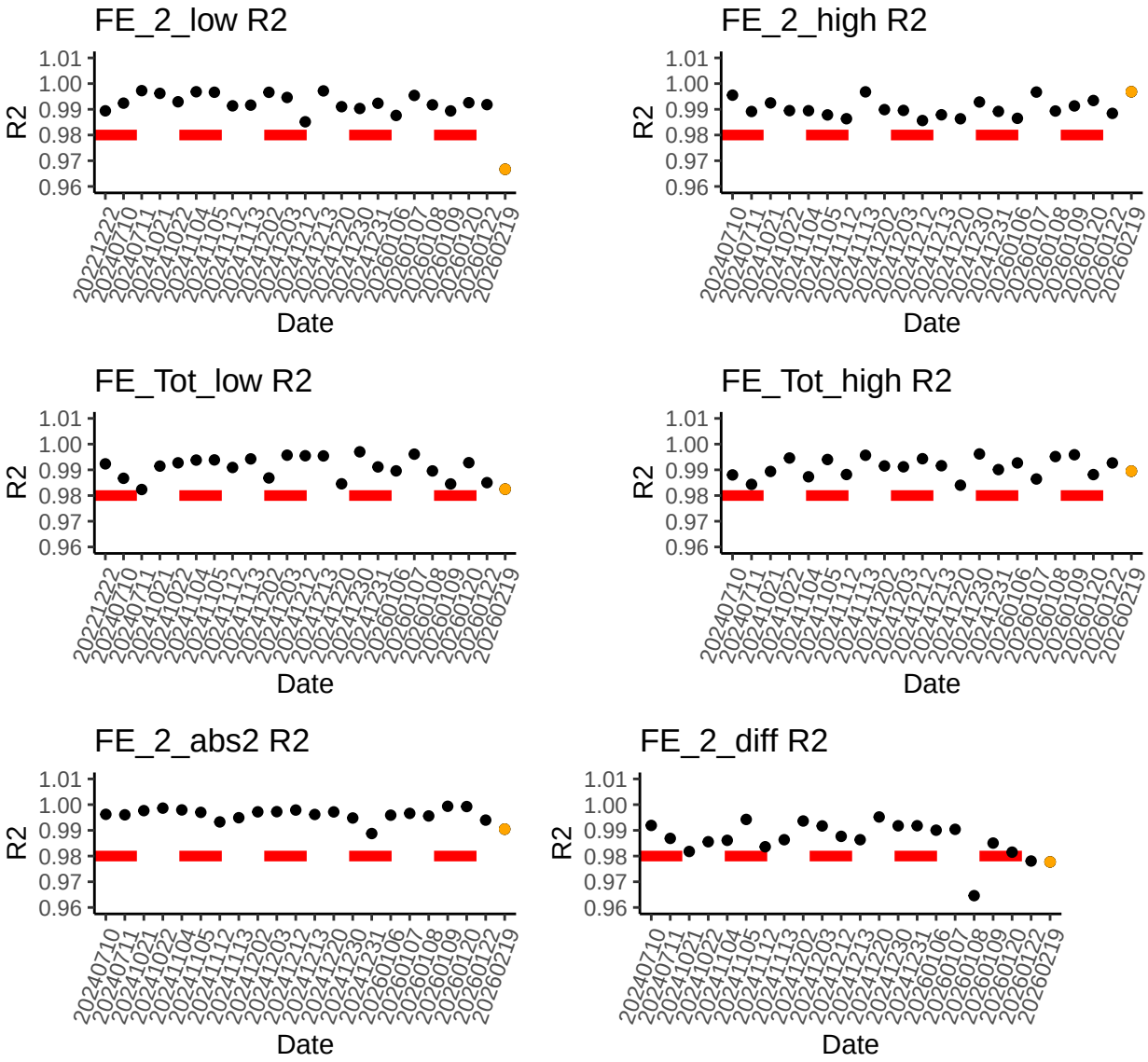
Date	Project	Curve	R2	Slope	Intercept	Top_STD
20260219	TEMPEST	FE_2_low	0.9666749	0.0027477	0.0471615	60
20260219	TEMPEST	FE_2_high	0.9968361	0.0021470	0.0567124	500
20260219	TEMPEST	FE_Tot_low	0.9824936	0.0016906	0.0425620	60
20260219	TEMPEST	FE_Tot_high	0.9894879	0.0016386	0.0431289	100
20260219	TEMPEST	FE_2_abs2	0.9904810	0.0038901	0.0518193	100
20260219	TEMPEST	FE_3_abs1	0.0277115	0.0000046	0.0412449	500
20260219	TEMPEST	FE_2_diff	0.9777247	0.0014025	0.0018435	100


Low Fe(II) Absorbar
STD
Abs1
0.20
0.15
0.10
0.05
0
20
40
60
Conc_uM
High Fe(II) Absorban
STD
Abs1
0.9
0.6
0.3
0.0
0
100
200
300
400
500
Conc_uM
Fe(II) Absorbance 2
STD
Abs2
0.4
0.3
0.2
0.1
0
25
50
75
100
Conc_uM
Fe(II) Absorbance D
STD
FE_2_Diff
0.15
0.10
0.05
0.00
0
25
50
75
100
Conc_uM
Low Fe(III) Absorba
STD
Abs2
0.12
0.09
0.06
0
20
40
60
Conc_uM
High Fe(III) Absorba
STD
Abs2
0.20
0.15
0.10
0.05
0
25
50
75
100
Conc_uM

Fe(III) Absorbance 1 Curve
STD
Abs1
0.0500
0.0475
0.0450
0.0425
0.0400
0.0375
0
100
200
300
400
500
Conc_uM

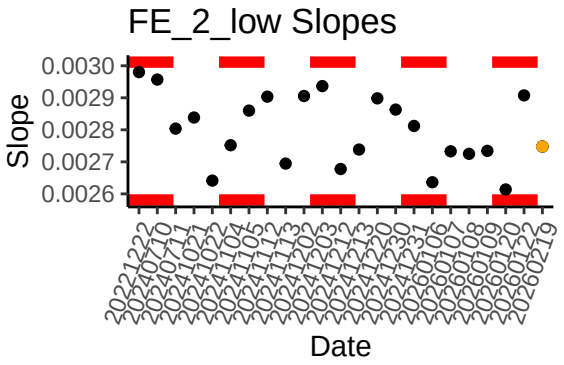
Checking STD Data against QAQC file

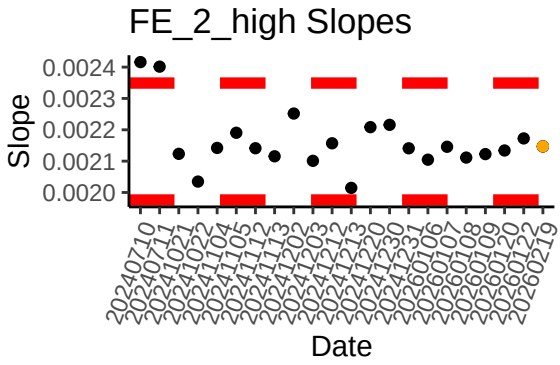
R2

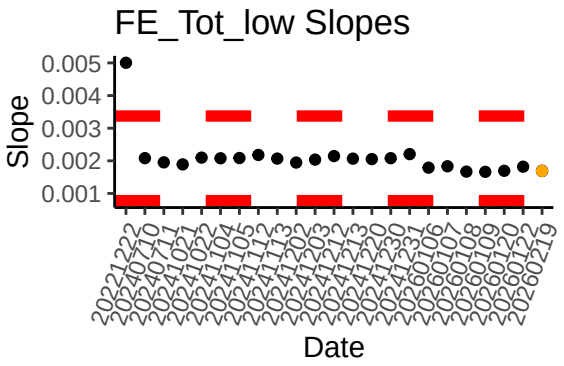


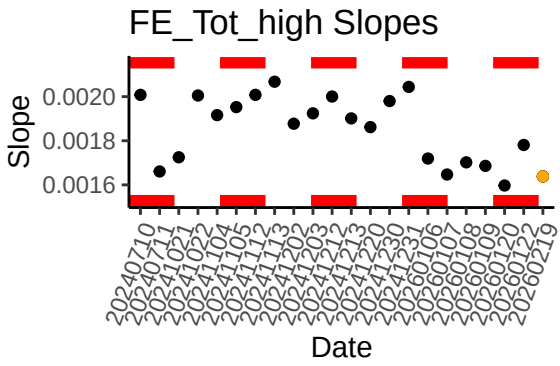

```
## [1] "FE_2_low: Std Curve r2 is below cutoff! - REASSESS"
## [1] "FE_2_high: Std Curve r2 GOOD"
## [1] "FE_Tot_low: Std Curve r2 is below cutoff! - REASSESS"
## [1] "FE_Tot_high: Std Curve r2 GOOD"
## [1] "FE_2_abs2: Std Curve r2 GOOD"
## [1] "FE_3_abs1: R2 will always be low"
## [1] "FE_2_diff: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

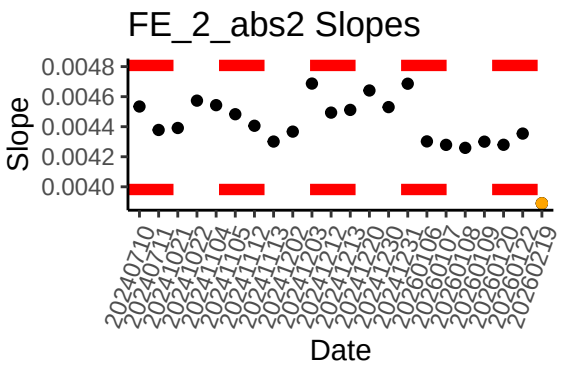
Slopes

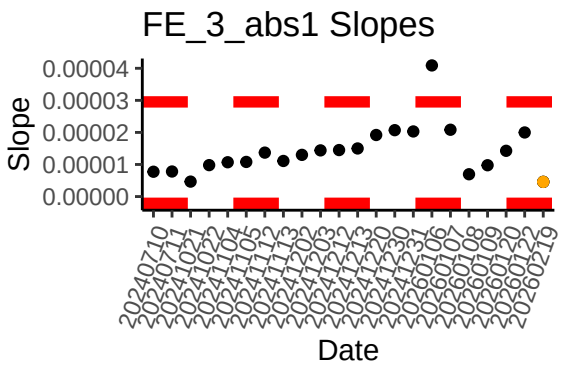


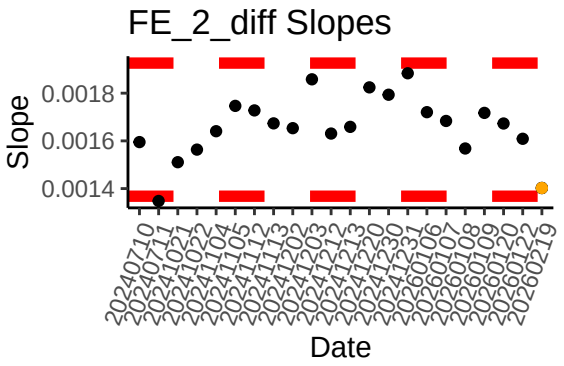








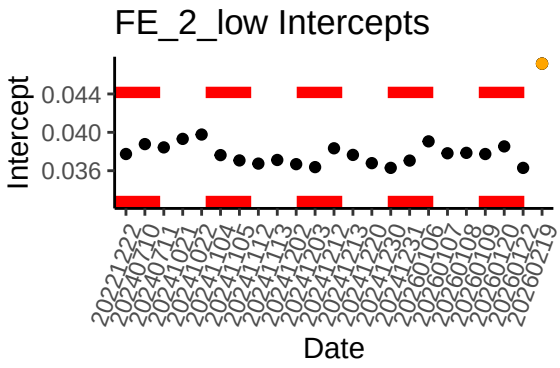


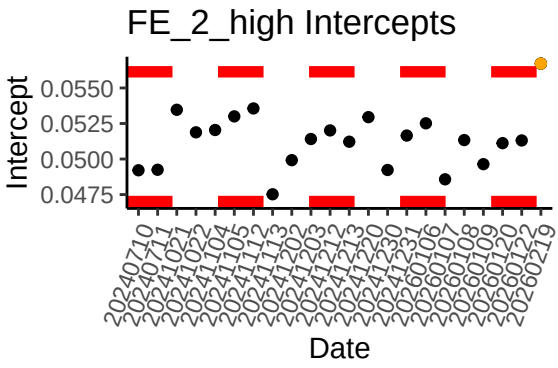


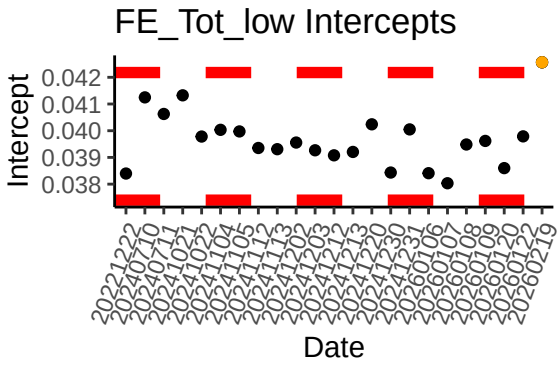

```
## [1] "FE_2_low:Std curve slope is with 2 sd of previous slopes"
## [1] "FE_2_high:Std curve slope is with 2 sd of previous slopes"
```

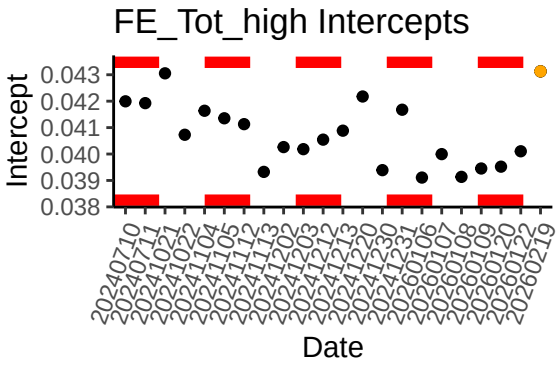
```
## [1] "FE_Tot_low:Std curve slope is with 2 sd of previous slopes"
## [1] "FE_Tot_high:Std curve slope is with 2 sd of previous slopes"
## [1] "FE_2_abs2: Std curve slope is 2 sd different from previous slopes! \n      - REASSESS"
## [1] "FE_3_abs1:Std curve slope is with 2 sd of previous slopes"
## [1] "FE_2_diff:Std curve slope is with 2 sd of previous slopes"
```

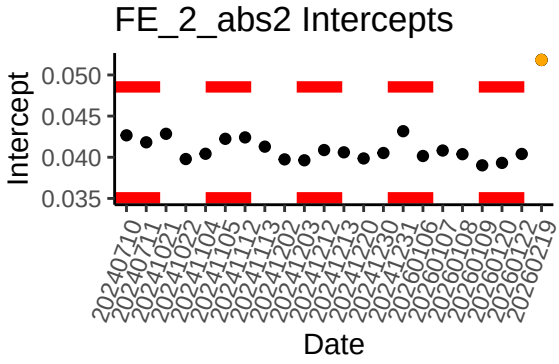
Intercepts

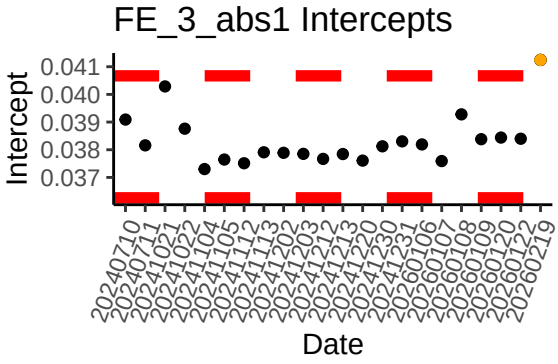


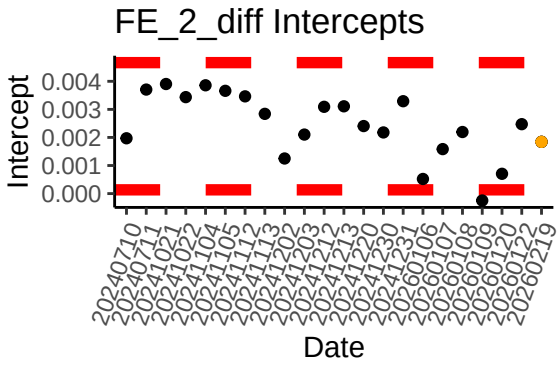










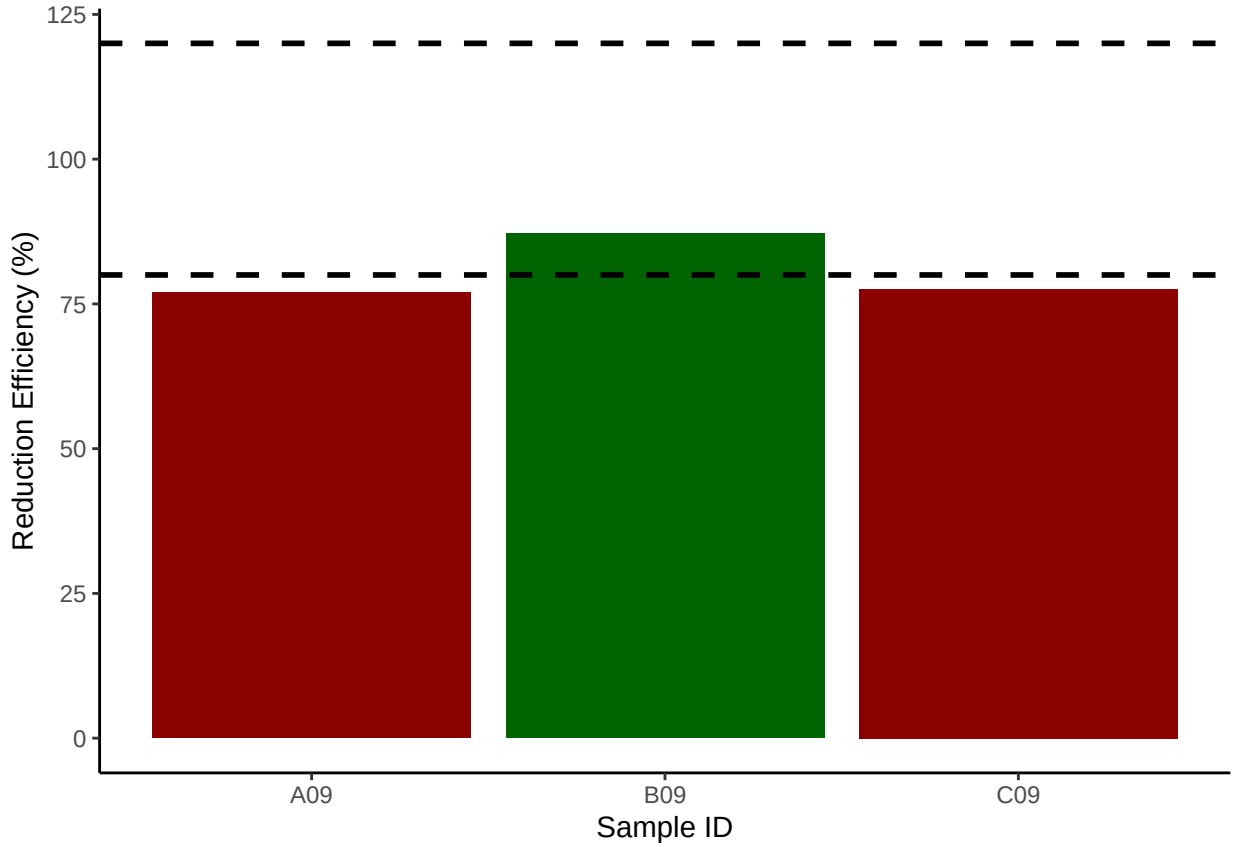



```
## [1] "FE_2_low:Std curve intercept is 2 sd different from previous intercepts! \n      - REASSESS"
## [1] "FE_2_high:Std curve intercept is 2 sd different from previous intercepts! \n      - REASSESS"
## [1] "FE_Tot_low:Std curve intercept is 2 sd different from previous intercepts! \n      - REASSESS"
## [1] "FE_Tot_high:Std curve intercept is with 2 sd of previous intercepts"
## [1] "FE_2_abs2:Std curve intercept is 2 sd different from previous intercepts! \n      - REASSESS"
## [1] "FE_3_abs1:Std curve intercept is 2 sd different from previous intercepts! \n      - REASSESS"
## [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	0.234	0.144	61.53846	76.92308	NO, rerun
B09	0.198	0.138	69.69697	87.12121	OK
C09	0.224	0.139	62.05357	77.56696	NO, rerun




```
## [1] "<60% of Reduction Efficiencies are out of range - REASSESS"
```

Method Minimum Detection Limit (MDL) Calculation

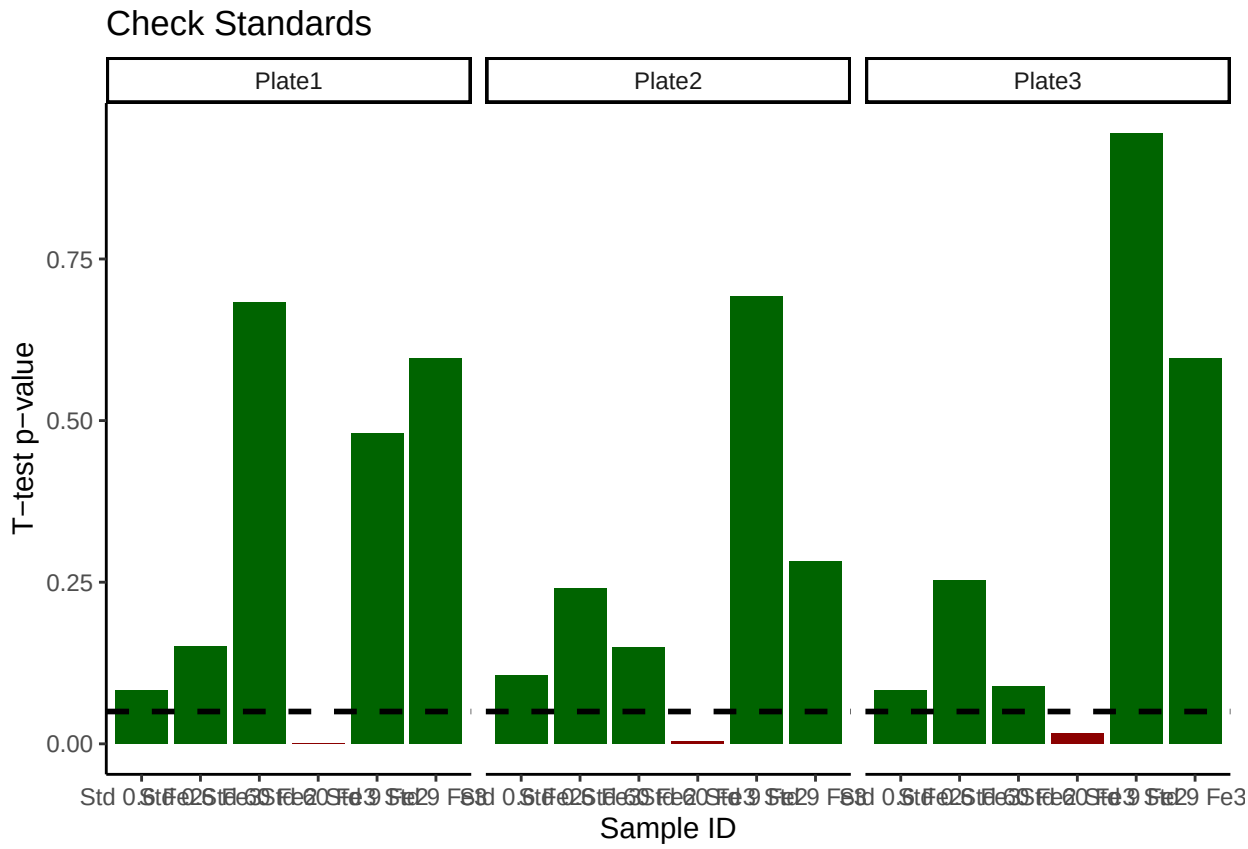
I use the lowest standard to calculate MDL How to calculate MDL https://www.epa.gov/sites/default/files/2016-12/documents/mdl-procedure_rev2_12-13-2016.pdf Look at Table 1 on page 5 The Student's t-value used to calculate the method detection limit (MDL) is the one appropriate for a 99% confidence level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

```
## [1] 0.03296242
```

Check standards QAQC

```
## [1] "Plate1"
## [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 is signficantly different from Std - REASSESS"
## [1] "Plate2"
## [1] "Fe2 Chk Std 0.6 GOOD"
## [1] "Fe2 Chk Std 9 GOOD"
```

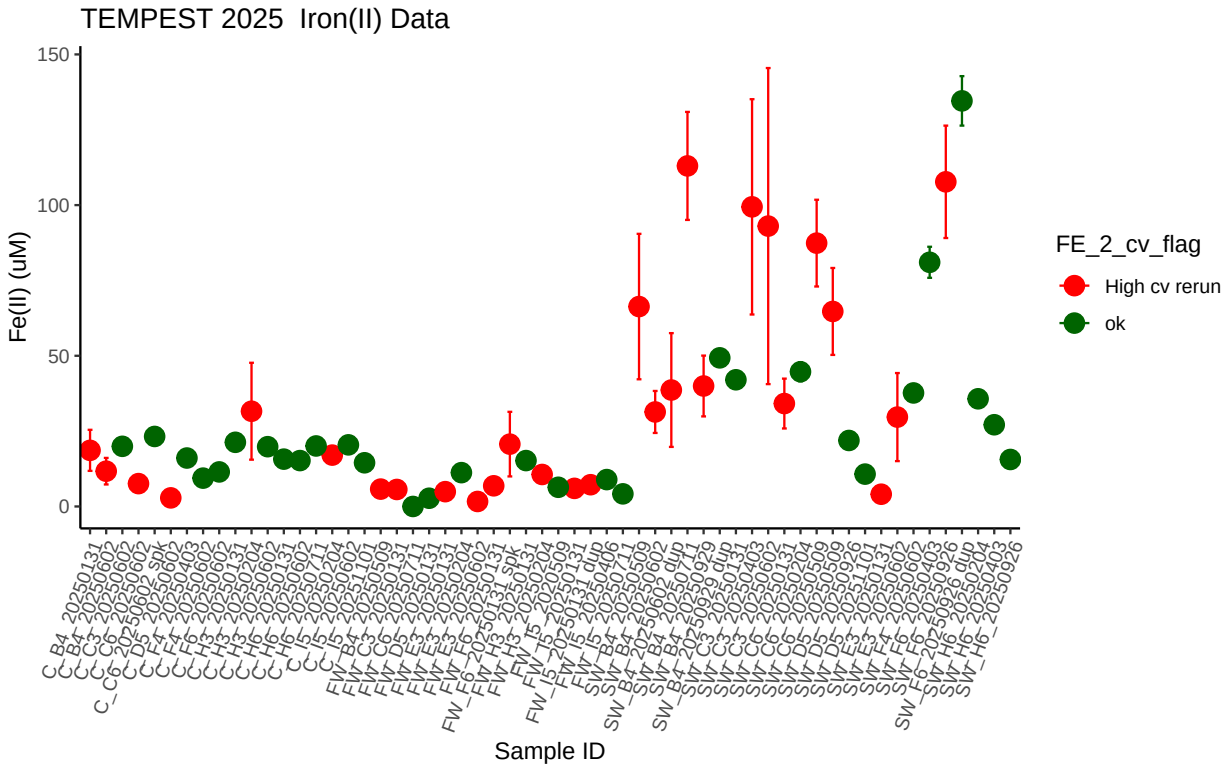
```
## [1] "Fe2 Chk Std 60 GOOD"
## [1] "Fe 3 Chk Std 0.6 Fe2 GOOD"
## [1] "Fe 3 Chk Std 9 GOOD"
## [1] "Fe 3 Chk Std 60 is signficantly different from Std - REASSESS"
## [1] "Plate3"
## [1] "Fe2 Chk Std 0.6 GOOD"
## [1] "Fe2 Chk Std 9 GOOD"
## [1] "Fe2 Chk Std 60 GOOD"
## [1] "Fe 3 Chk Std 0.6 Fe2 GOOD"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

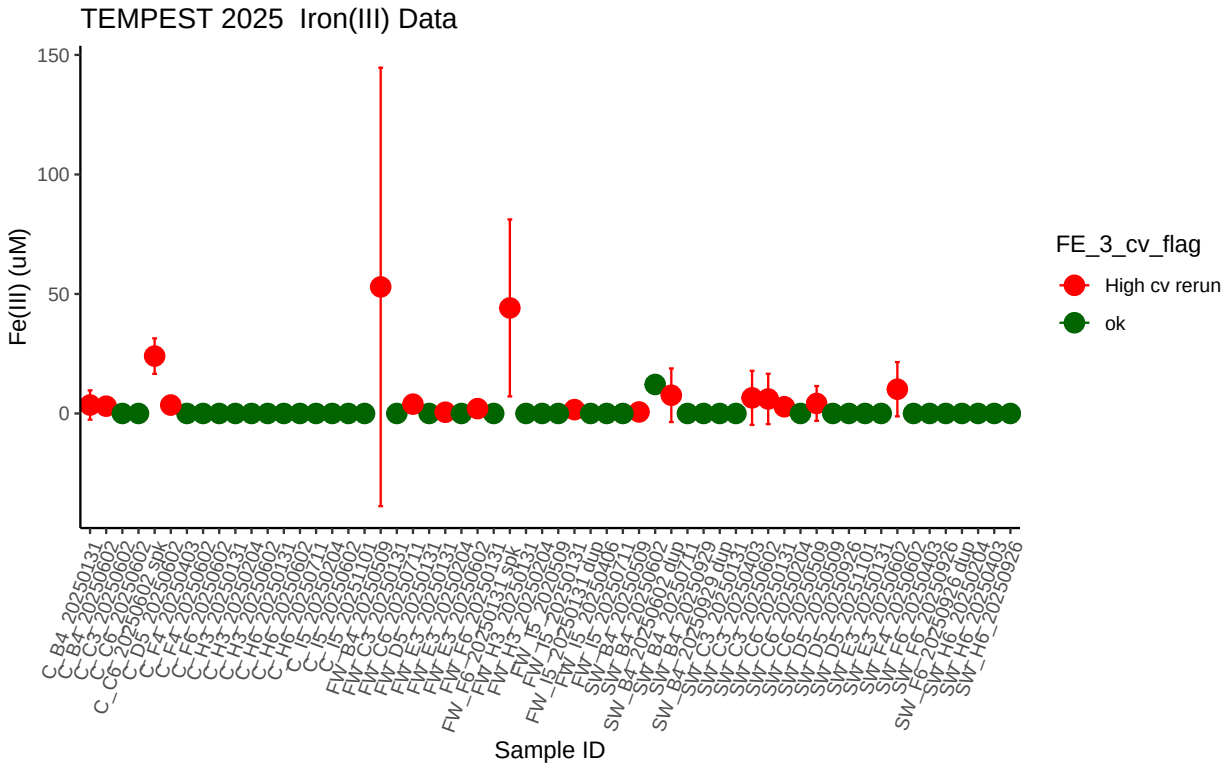


#No Matrix Checks We do not use matrix checks for the Fe samples because our matrix checks are not made with Trace metal grade reagents. If we want to do this in the future, we need to use trace metal grade sodium chloride and sodium bicarbonate for making the matrix checks

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	14.498700	0.000000	59.865688	59.273425	ok	High cv rerun
Plate1_1_FW_I5_20250131	7.219955	14.257291	0.000000	0.000000	High cv rerun	ok
Plate1_1_SW_C3_20250403	119.135132	12.439934	0.000000	0.000000	High cv rerun	ok
Plate1_1_SW_C6_20250131	29.420127	5.248295	4.220049	51.912071	ok	High cv rerun
Plate2_1_C_B4_20250602	9.221610	13.953231	4.580882	69.141335	High cv rerun	High cv rerun
Plate2_1_C_C6_20250602 spk	23.233194	9.528367	20.077352	20.722634	ok	High cv rerun
Plate2_1_C_D5_20250602	3.762551	34.197876	5.297483	59.788457	High cv rerun	High cv rerun
Plate2_1_FW_E3_20250602	2.488771	20.680291	0.000000	0.000000	High cv rerun	ok
Plate2_1_SW_B4_20250602 dup	27.782409	8.336507	11.439514	111.947835	ok	High cv rerun
Plate2_1_SW_C3_20250602	13.807166	30.237313	0.000000	0.000000	High cv rerun	ok
Plate2_1_SW_E3_20250602	21.231539	3.636230	15.226086	66.700055	ok	High cv rerun
Plate1_1_FW_C3_20250131	6.310112	12.234768	0.000000	0.000000	High cv rerun	ok
Plate1_1_SW_E3_20250131	2.852708	18.041981	0.000000	0.000000	High cv rerun	ok
Plate2_1_SW_B4_20250602	35.061154	11.009727	12.141846	7.521552	High cv rerun	ok
Plate3_1_SW_F6_20250926	116.806341	12.124042	0.000000	0.000000	High cv rerun	ok

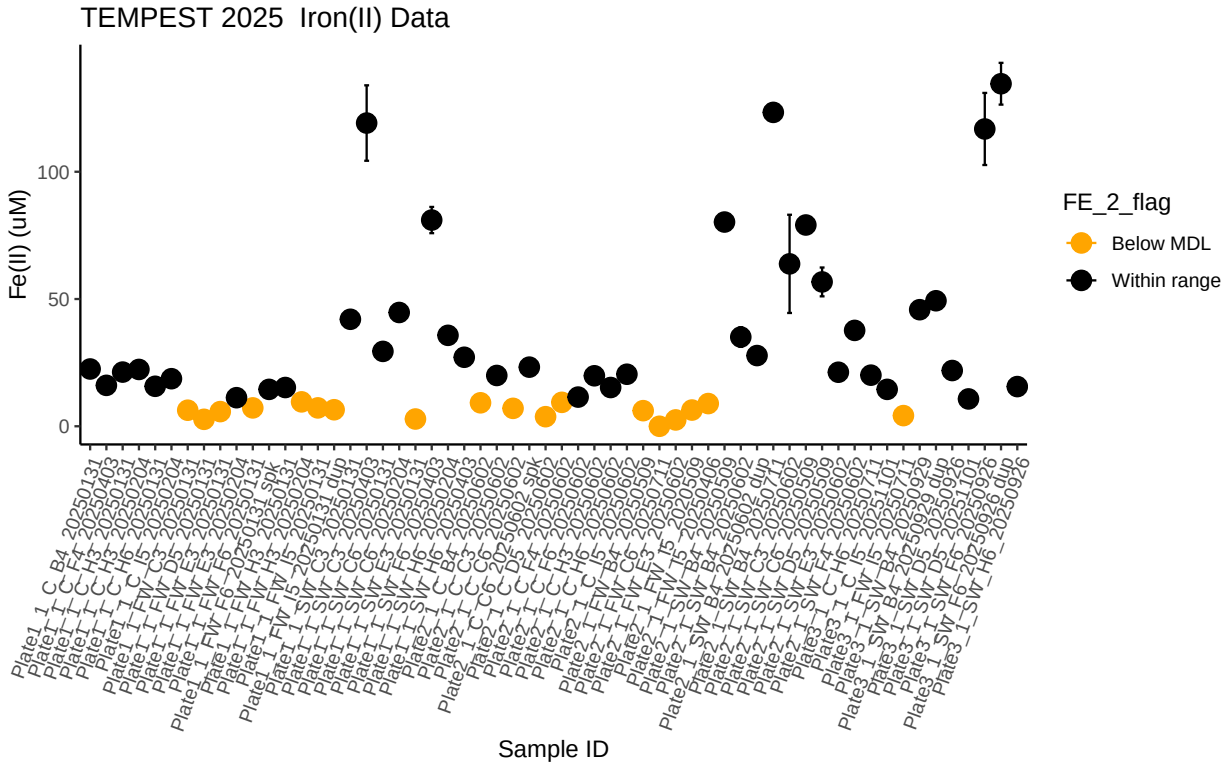
Table 4: Samples Above the Detection Limit that should be rerun at a higher dilution

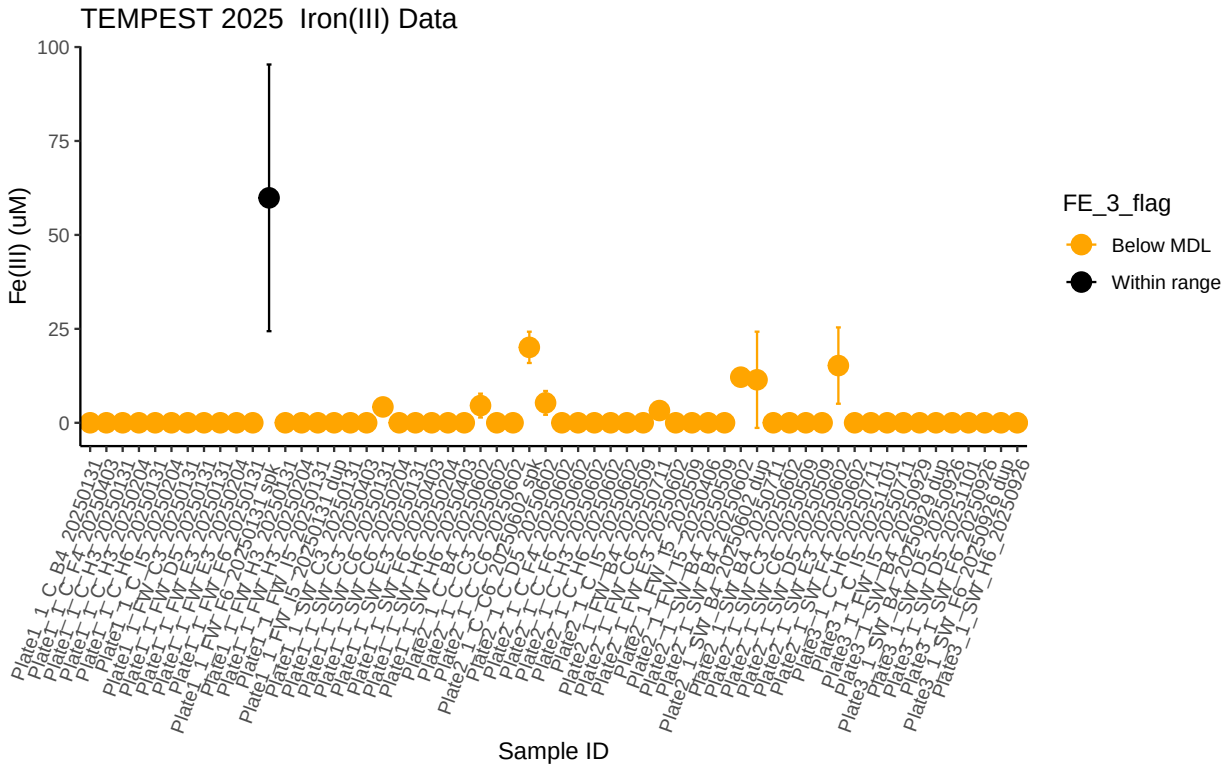
ID full	FE 2 mean	FE 3 mean	FE tot mean	FE 2 flag	FE 3 flag

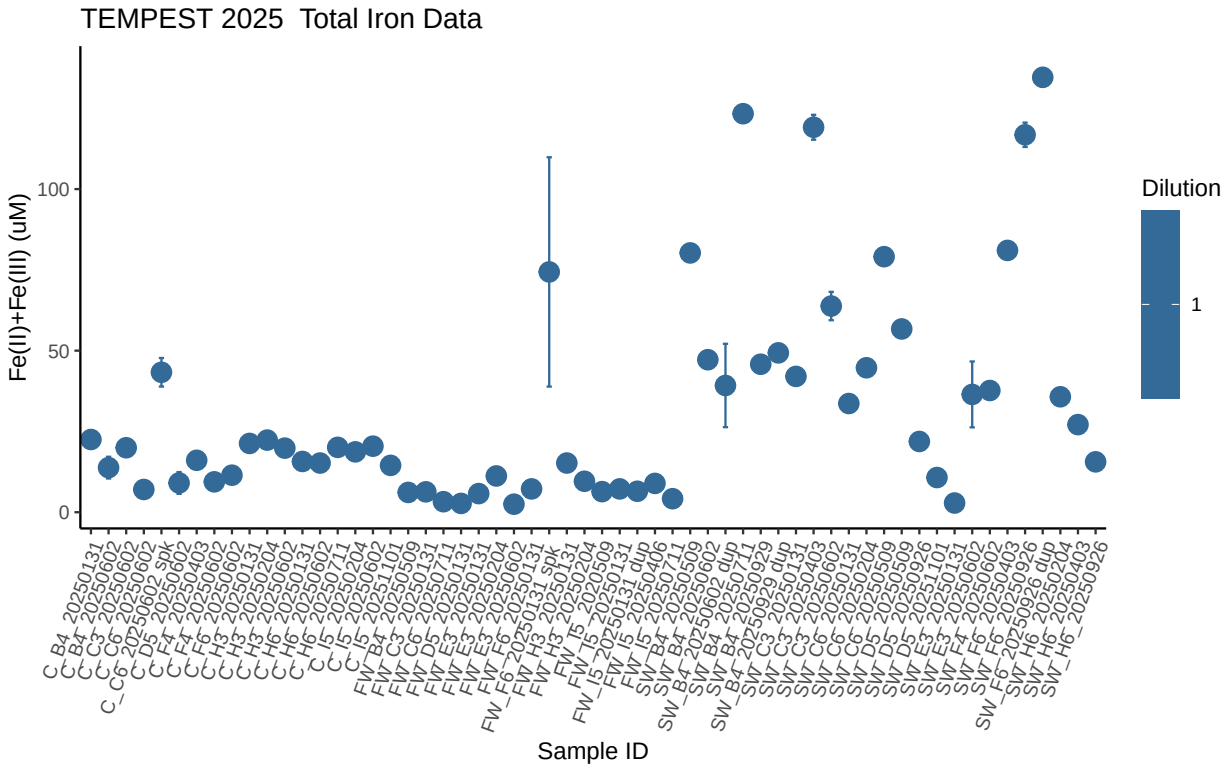
Table 5: Samples Below the Detection Limit that should be rerun at a lower dilution

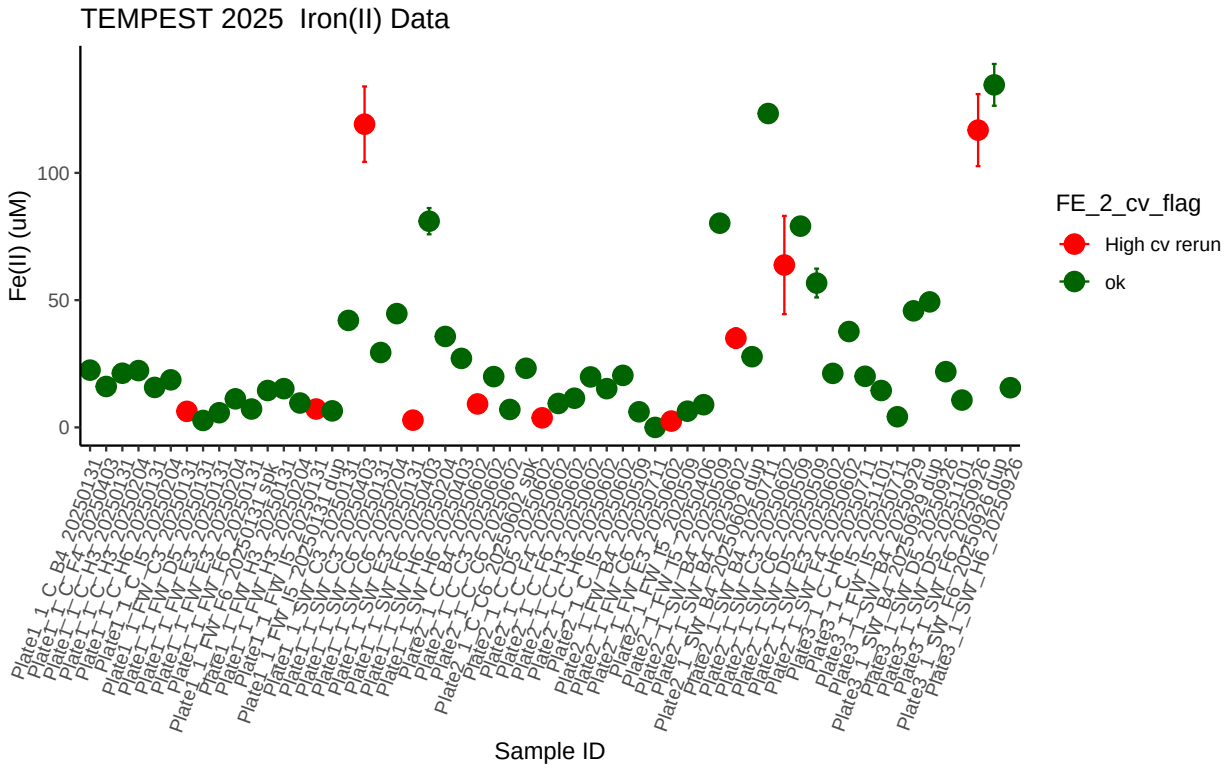
ID full	FE 2 mean	FE 3 mean	FE tot mean	FE 2 flag	FE 3 flag

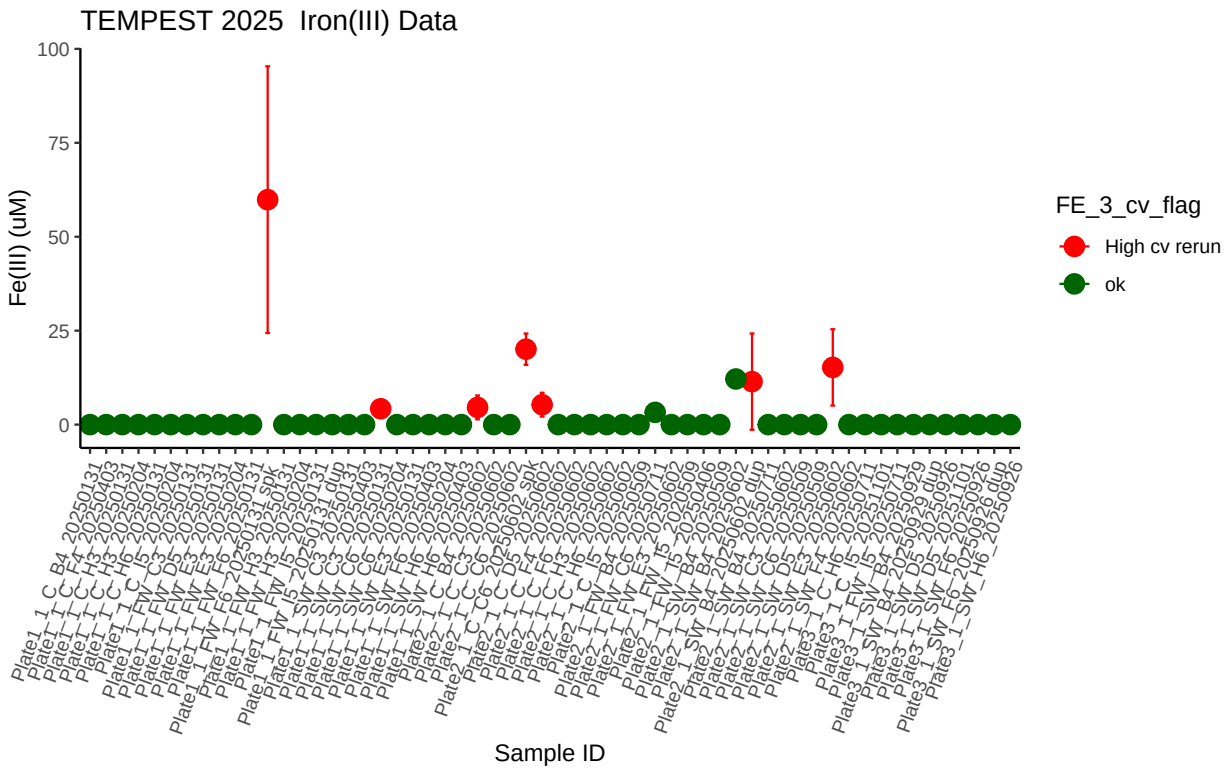
Plot data after bad reps were removed



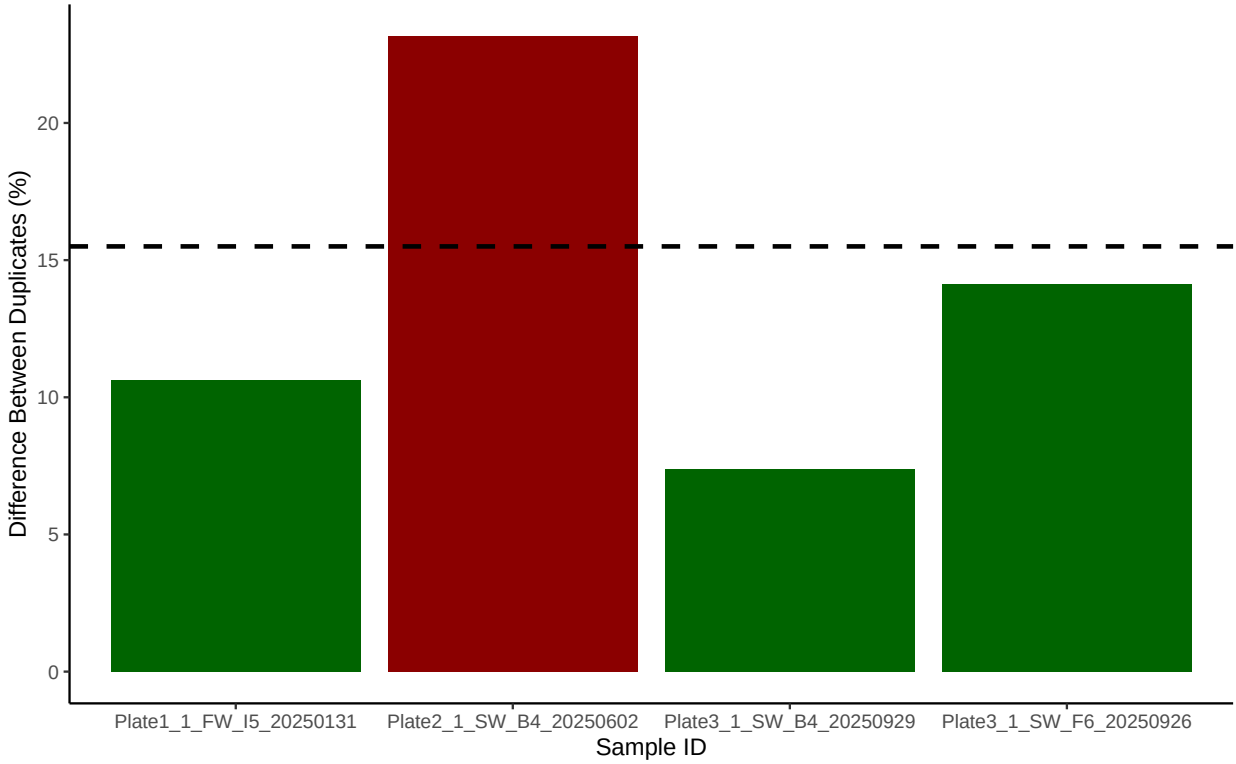


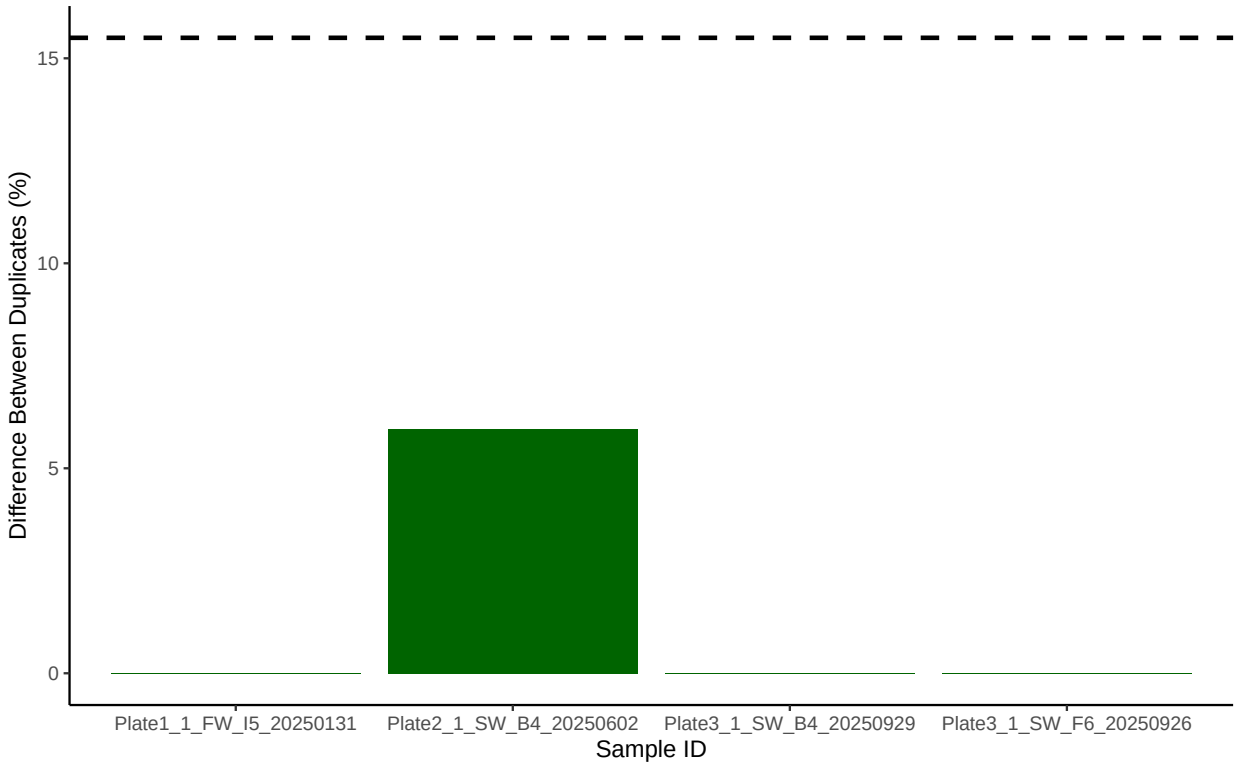

TEMPEST 2025 Total Iron Data
Fe(II)+Fe(III) (uM)
100
50
0
Dilution
1
Sample ID

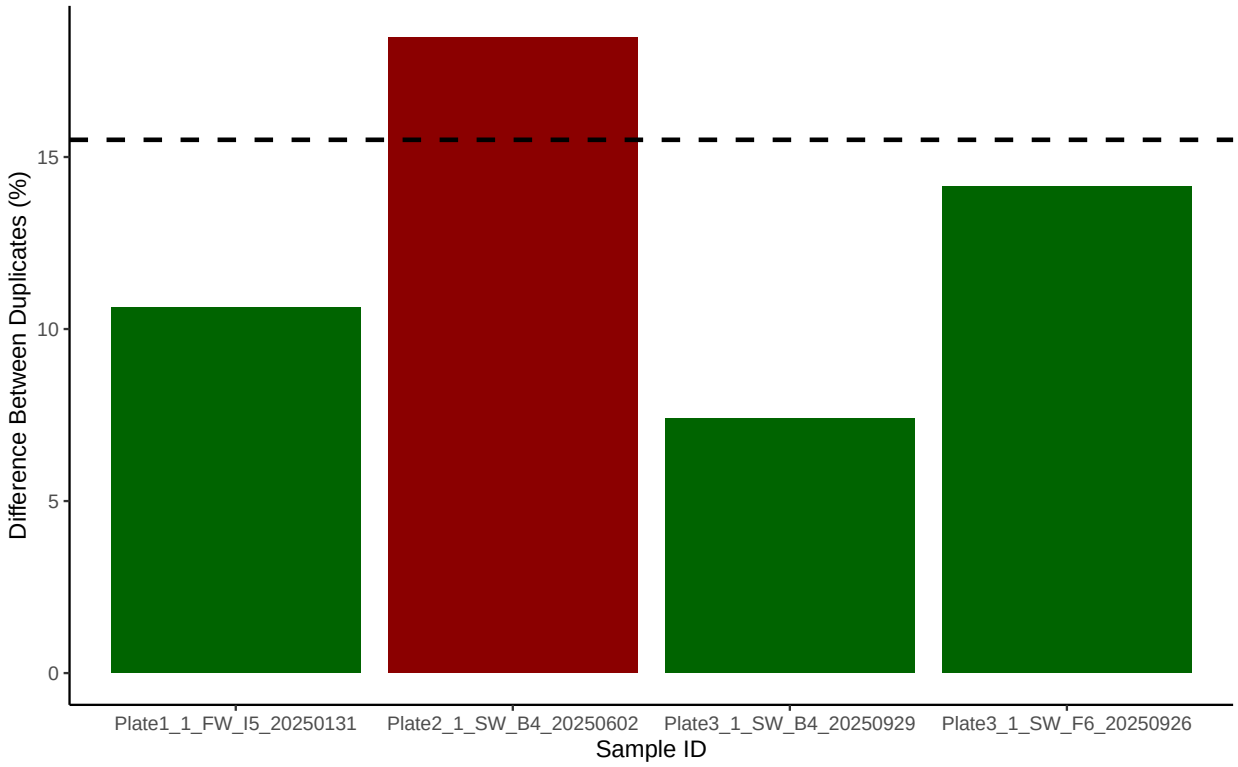

TEMPEST 2025 Iron(II) Data
Fe(II) (uM)
100
50
0
FE_2_cv_flag
High cv rerun
ok
Sample ID


TEMPEST 2025 Iron(III) Data
Fe(III) (uM)
100
75
50
25
0
Sample ID
FE_3_cv_flag
High cv rerun
ok

Check Dups for QAQC



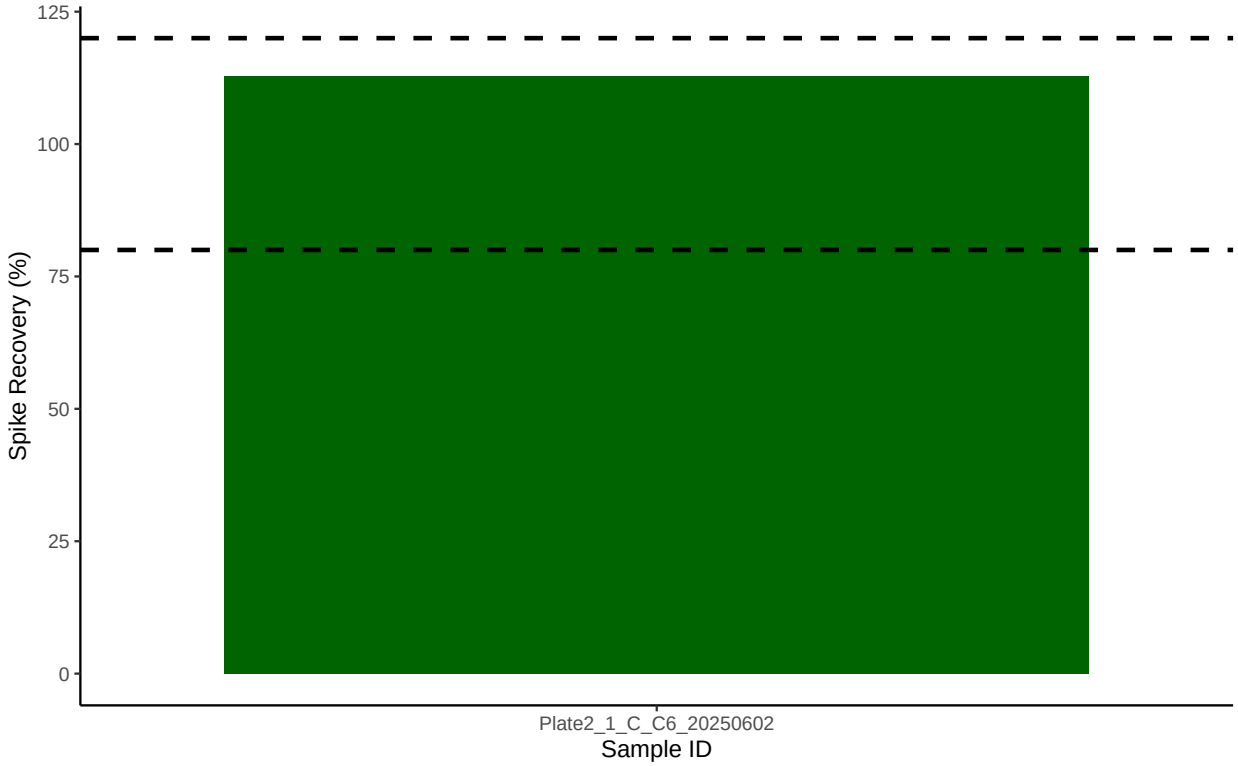





```
## [1] ">60% of Fe 2 Duplicates are within <10%"
```

```
## [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