FeCode_updated2025_20260219

2026-02-20

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"#any notes from run

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

File paths

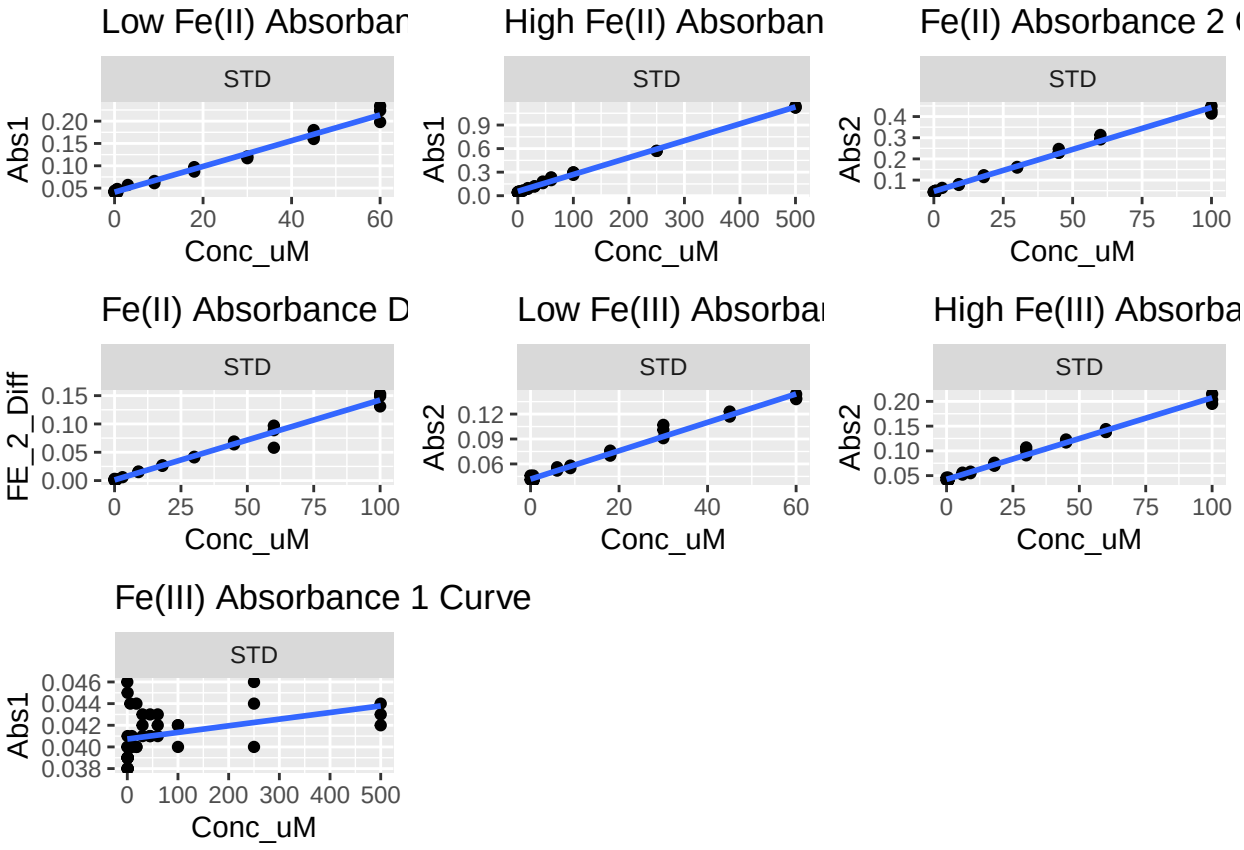
```
## [1] "Tidy Data/20260219_TEMPEST_Fe_STD.csv"
```

```
## [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

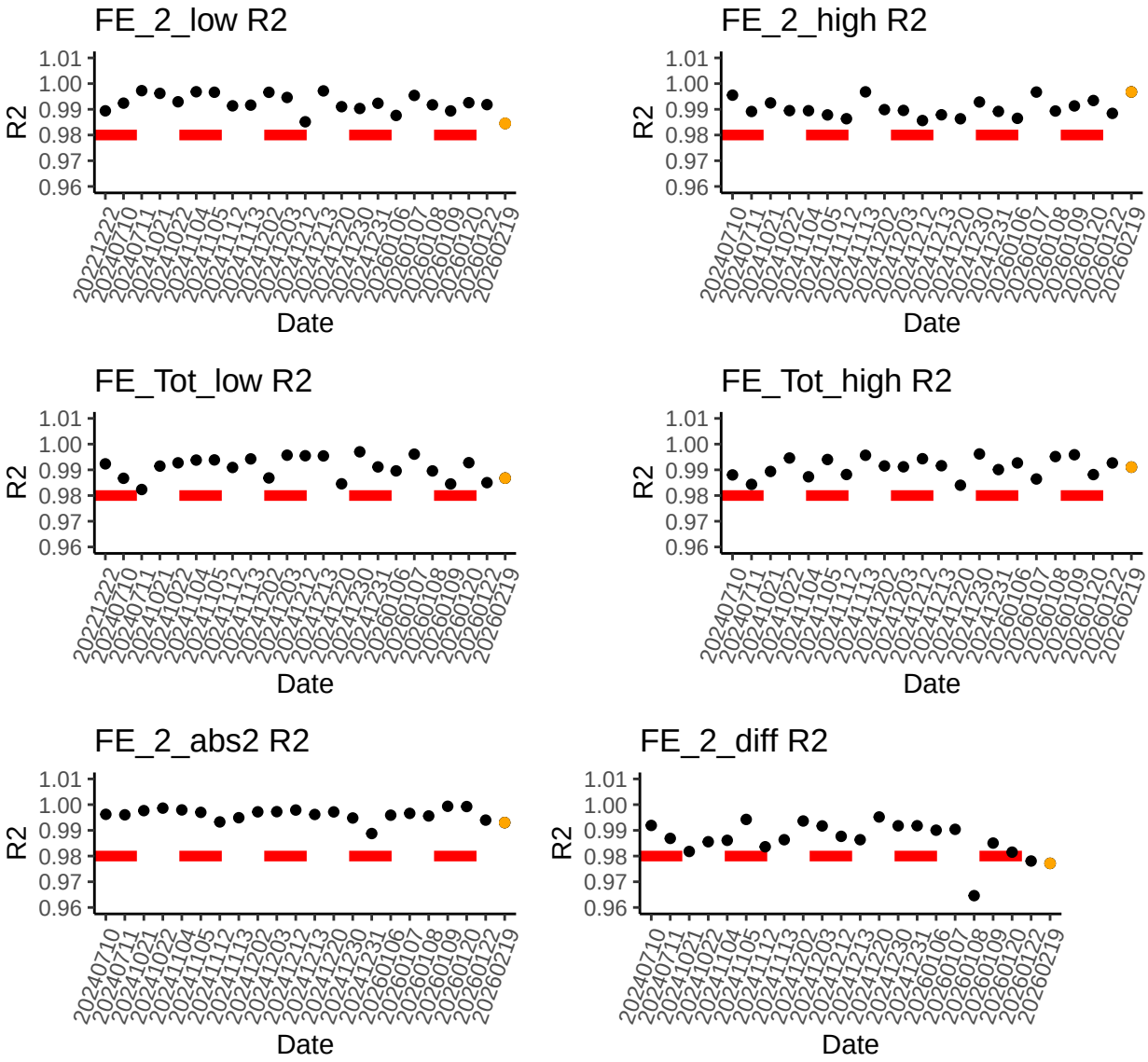
Date	Project	Curve	R2	Slope	Intercept	Top_STD
20260219	TEMPEST	FE_2_low	0.9845048	0.0028810	0.0409565	60
20260219	TEMPEST	FE_2_high	0.9967558	0.0021510	0.0553532	500
20260219	TEMPEST	FE_Tot_low	0.9867712	0.0017086	0.0417063	60
20260219	TEMPEST	FE_Tot_high	0.9910473	0.0016493	0.0423899	100
20260219	TEMPEST	FE_2_abs2	0.9930166	0.0039655	0.0465192	100
20260219	TEMPEST	FE_3_abs1	0.1263420	0.0000061	0.0407269	500
20260219	TEMPEST	FE_2_diff	0.9771476	0.0014118	0.0010988	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
0.046
0.044
0.042
0.040
0.038
0
100
200
300
400
500
Conc_uM

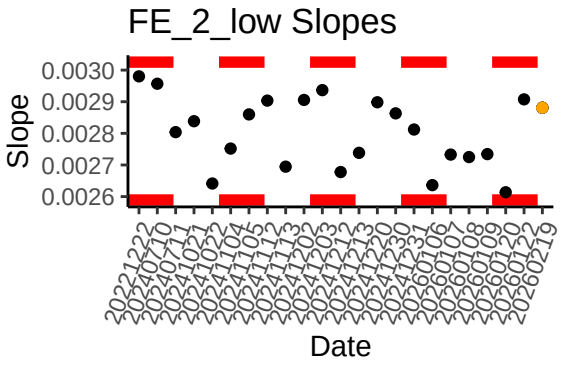
Checking STD Data against QAQC file

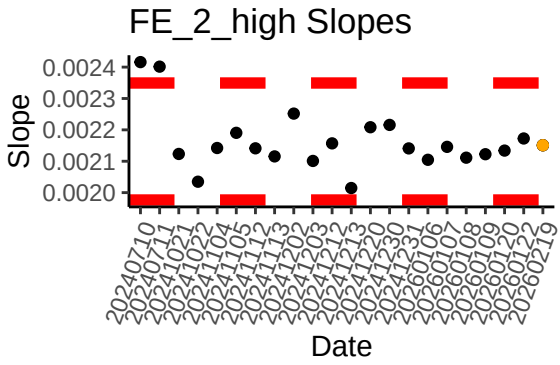
R2

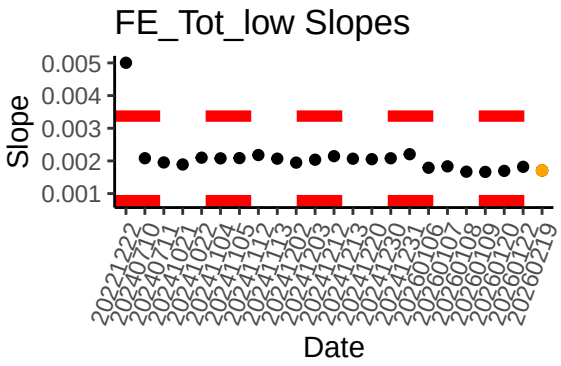


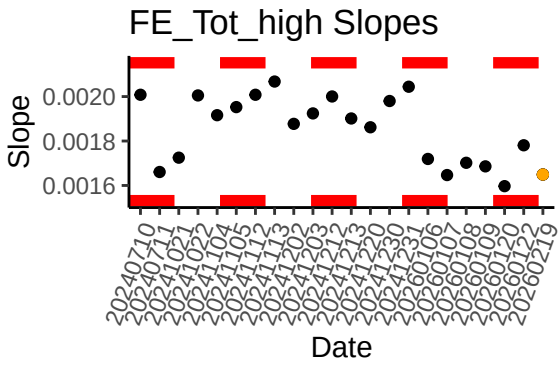

```
## [1] "FE_2_low: Std Curve r2 is below cutoff! - REASSESS"
## [1] "FE_2_high: Std Curve r2 GOOD"
## [1] "FE_Tot_low: Std Curve r2 GOOD"
## [1] "FE_Tot_high: Std Curve r2 GOOD"
## [1] "FE_2_abs2: Std Curve r2 GOOD"
## [1] "FE_3_abs1: R2 will always be low"
## [1] "FE_2_diff: Std Curve r2 is below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

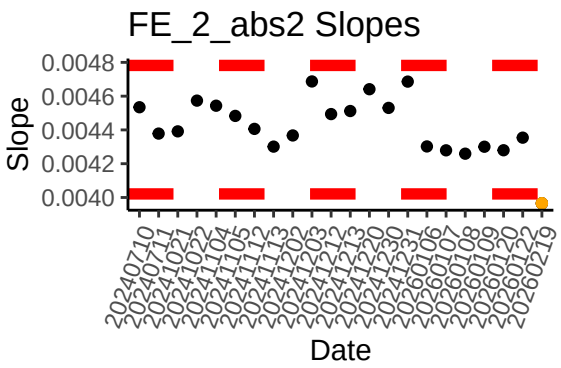
Slopes

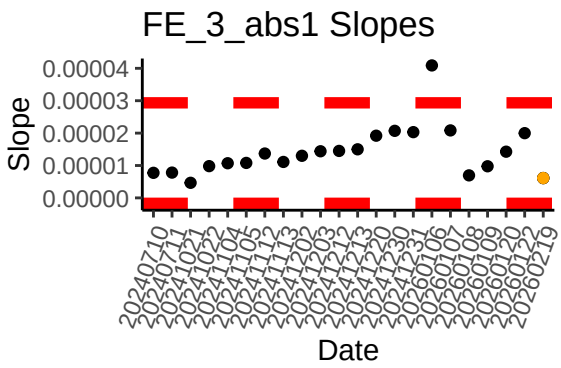


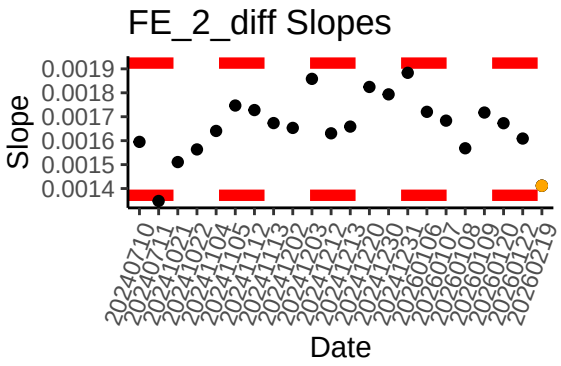








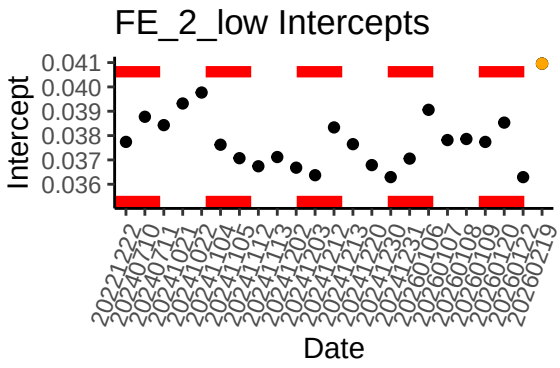


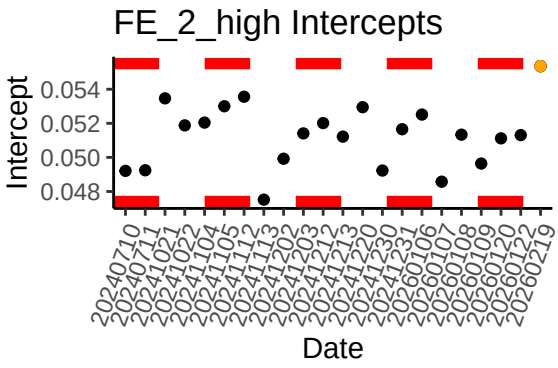


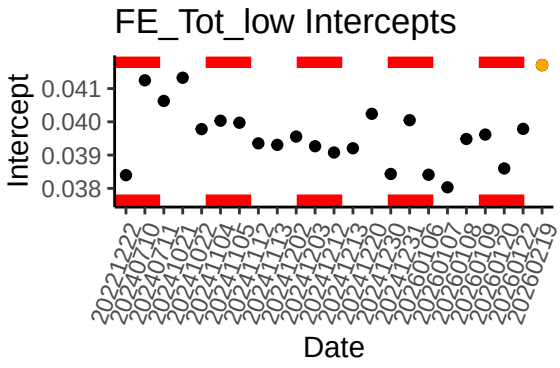

```
## [1] "FE_2_low:Std curve slope is with 2 sd of previous slopes"
## [1] "FE_2_high:Std curve slope is with 2 sd of previous slopes"
```

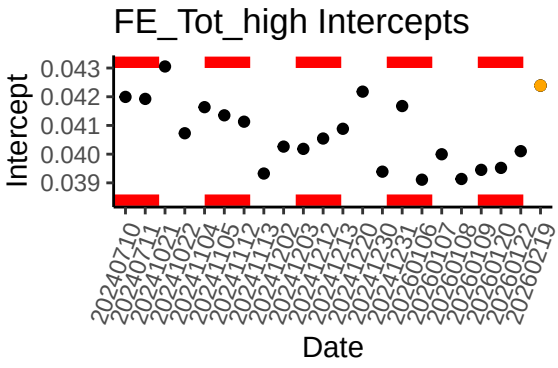
```
## [1] "FE_Tot_low:Std curve slope is with 2 sd of previous slopes"
## [1] "FE_Tot_high:Std curve slope is with 2 sd of previous slopes"
## [1] "FE_2_abs2: Std curve slope is 2 sd different from previous slopes! \n      - REASSESS"
## [1] "FE_3_abs1:Std curve slope is with 2 sd of previous slopes"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

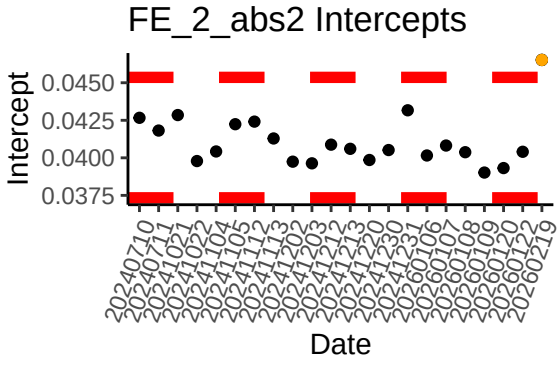
Intercepts

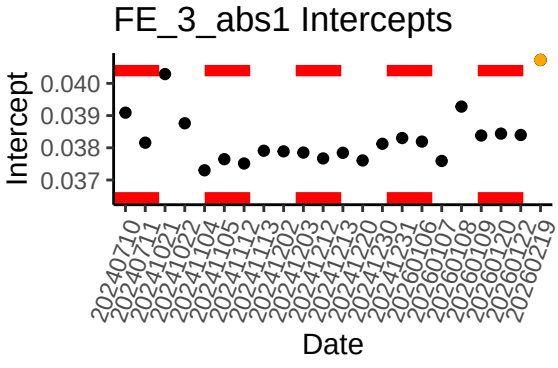


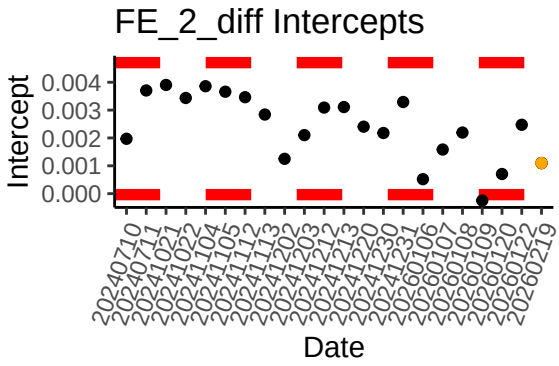










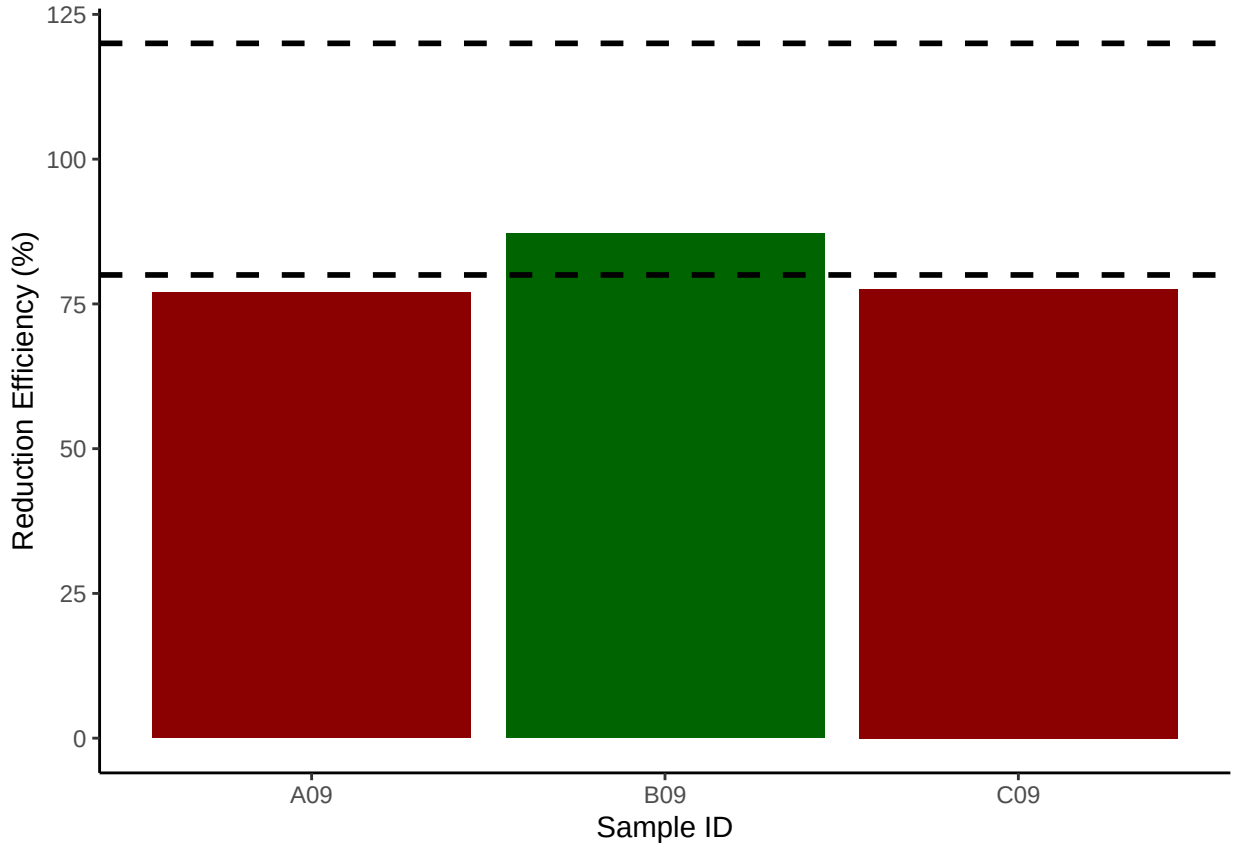



```
## [1] "FE_2_low:Std curve intercept is 2 sd different from previous intercepts! \n      - REASSESS"
## [1] "FE_2_high:Std curve intercept is with 2 sd of previous intercepts"
## [1] "FE_Tot_low:Std curve intercept is with 2 sd of previous intercepts"
## [1] "FE_Tot_high:Std curve intercept is with 2 sd of previous intercepts"
## [1] "FE_2_abs2:Std curve intercept is 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

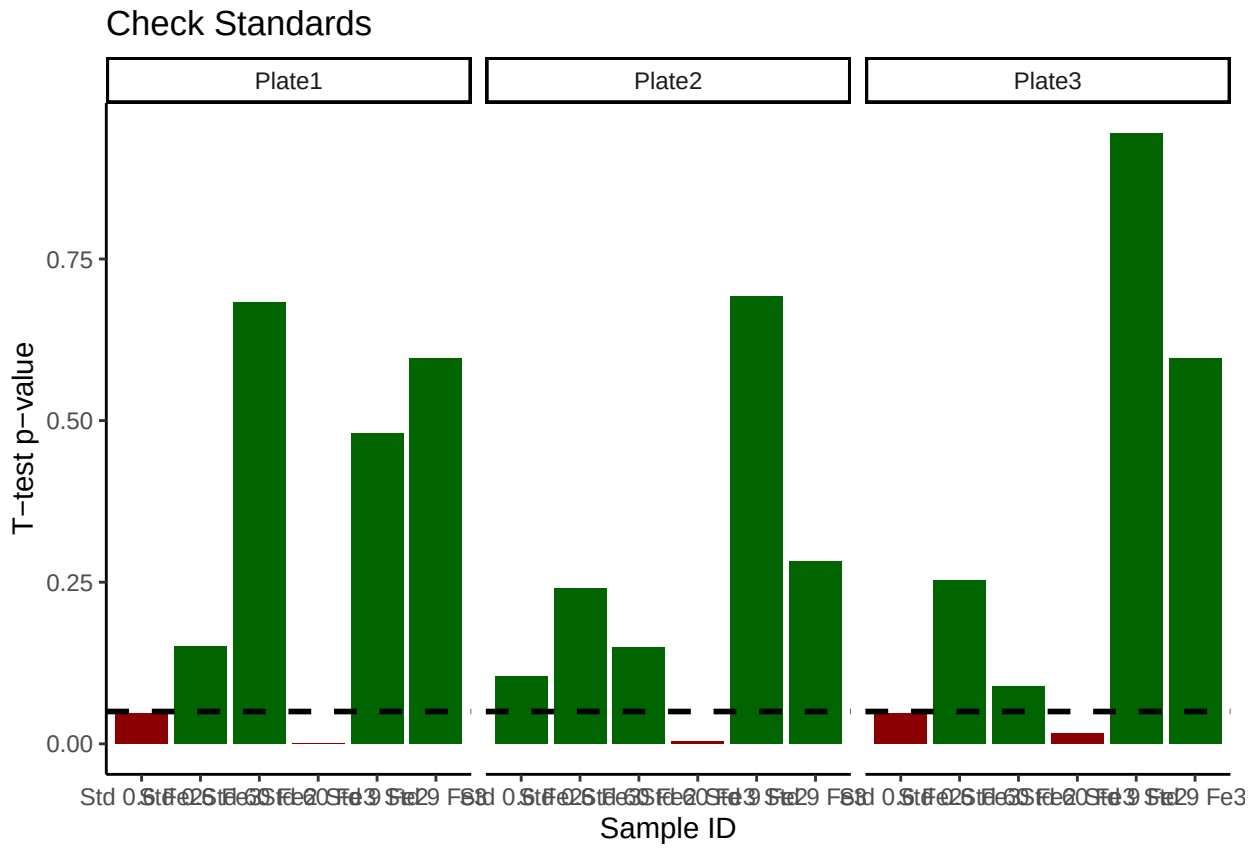
I use the lowest standard to calculate MDL How to calculate MDL https://www.epa.gov/sites/default/files/2016-12/documents/mdl-procedure_rev2_12-13-2016.pdf Look at Table 1 on page 5 The Student's t-value used to calculate the method detection limit (MDL) is the one appropriate for a 99% confidence level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

```
## [1] 0.01051597
```

Check standards QAQC

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

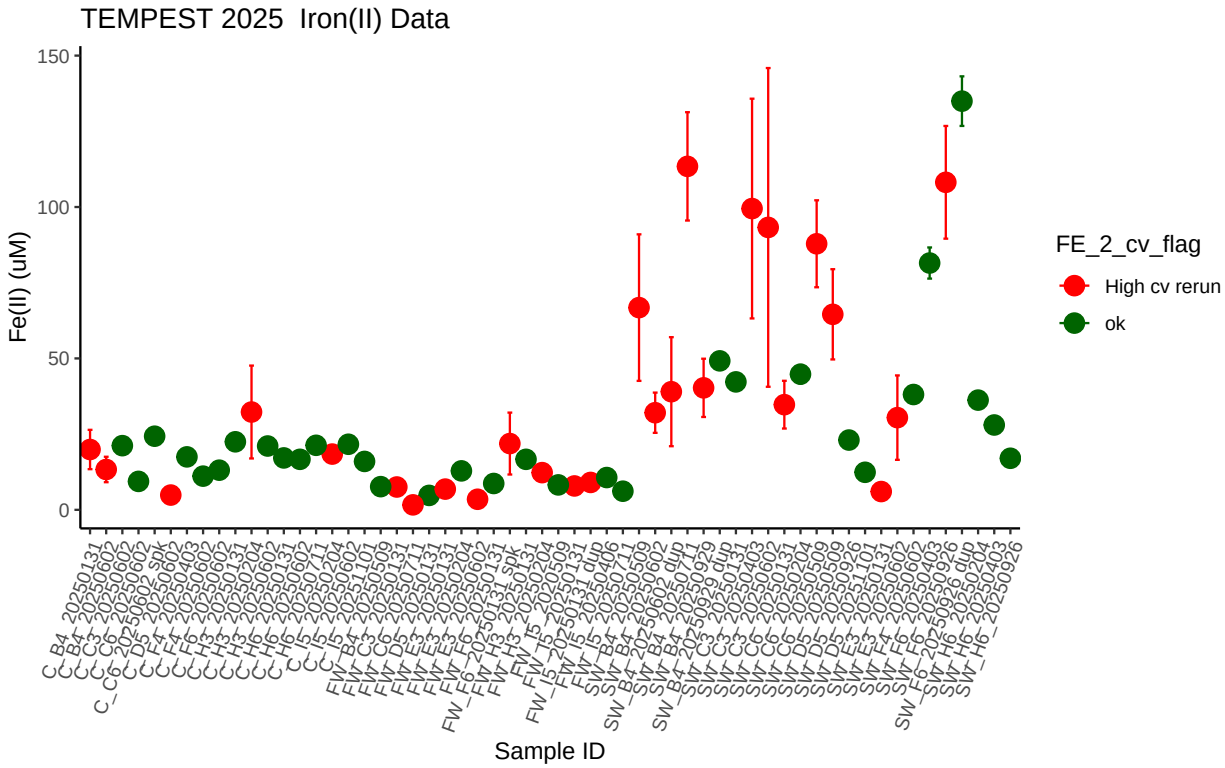
```
## [1] "Fe2 Chk Std 60 GOOD"
## [1] "Fe 3 Chk Std 0.6 Fe2 GOOD"
## [1] "Fe 3 Chk Std 9 GOOD"
## [1] "Fe 3 Chk Std 60 is signficantly different from Std - REASSESS"
## [1] "Plate3"
## [1] "Fe2 Chk Std 0.6 is signficantly different from Std - REASSESS"
## [1] "Fe2 Chk Std 9 GOOD"
## [1] "Fe2 Chk Std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

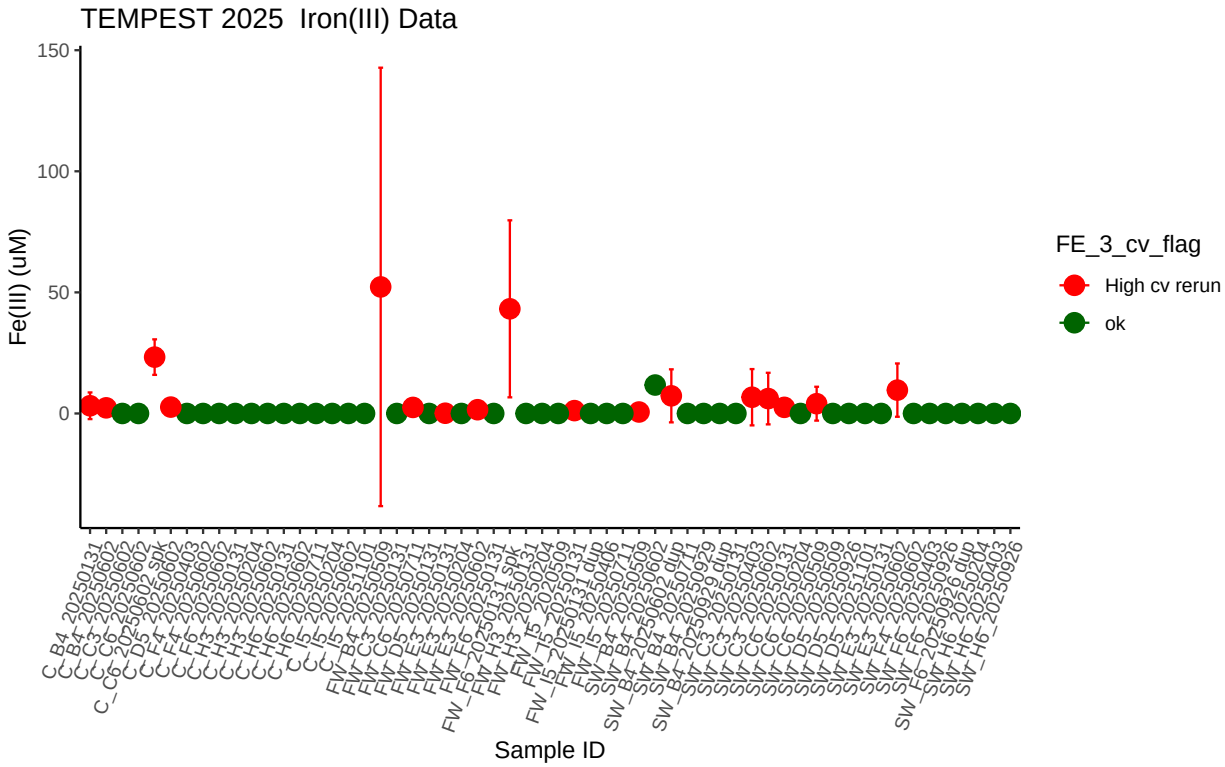


#No Matrix Checks We do not use matrix checks for the Fe samples because our matrix checks are not made with Trace metal grade reagents. If we want to do this in the future, we need to use trace metal grade sodium chloride and sodium bicarbonate for making the matrix checks

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	15.981862	0.000000	58.630674	60.186934	ok	High cv rerun
Plate1_1_FW_I5_20250131	9.039793	10.860390	0.000000	0.000000	High cv rerun	ok
Plate1_1_SW_C3_20250403	19.544952	12.374179	0.000000	0.000000	High cv rerun	ok
Plate1_1_SW_C6_20250131	30.213103	4.874161	3.801243	55.929164	ok	High cv rerun
Plate2_1_C_B4_20250602	10.948862	11.208434	3.491038	88.637400	High cv rerun	High cv rerun
Plate2_1_C_C6_20250602 spk	24.312345	8.684263	19.378652	20.853463	ok	High cv rerun
Plate2_1_C_D5_20250602	5.742310	21.371120	3.961468	78.111563	High cv rerun	High cv rerun
Plate2_1_FW_C6_20250711	1.924172	12.755572	1.870564	10.880918	High cv rerun	High cv rerun
Plate2_1_FW_E3_20250602	4.527448	10.842275	0.000000	0.000000	High cv rerun	ok
Plate2_1_SW_B4_20250602 dup	28.651138	7.709826	10.924969	115.849474	ok	High cv rerun
Plate2_1_SW_C3_20250602	3.967652	30.884472	0.000000	0.000000	High cv rerun	ok
Plate2_1_SW_E3_20250602	22.403276	3.286652	14.467484	69.990594	ok	High cv rerun
Plate1_1_SW_E3_20250131	4.874552	10.070227	0.000000	0.000000	High cv rerun	ok
Plate2_1_SW_B4_20250602	35.593207	10.343513	11.745288	6.060922	High cv rerun	ok
Plate3_1_SW_F6_20250926	17.220502	12.058687	0.000000	0.000000	High cv rerun	ok

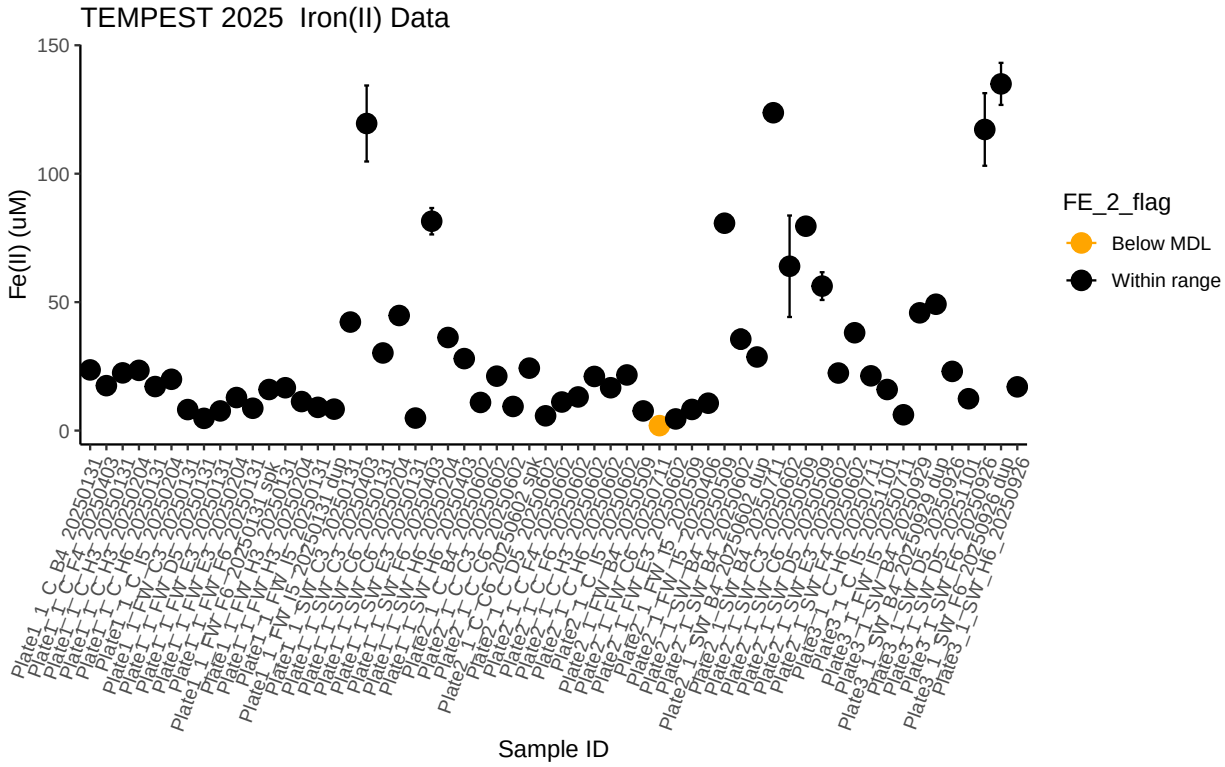
Table 4: Samples Above the Detection Limit that should be rerun at a higher dilution

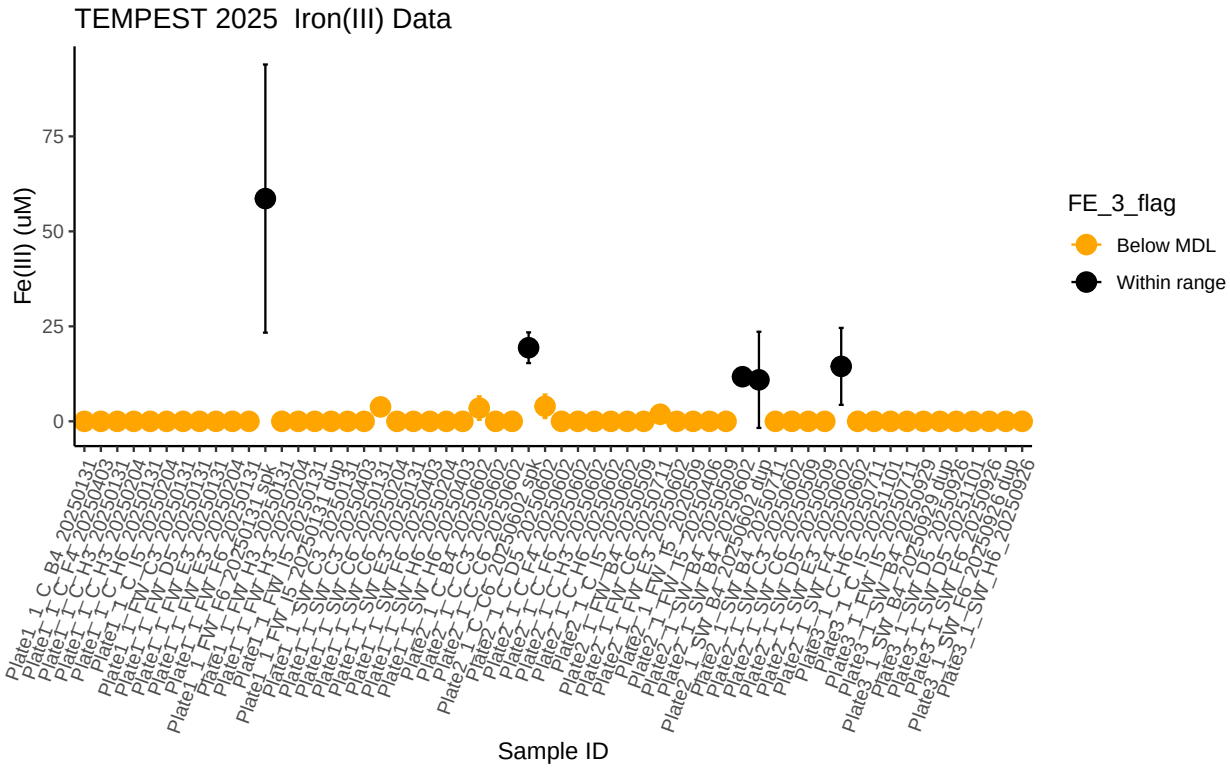
ID full	FE 2 mean	FE 3 mean	FE tot mean	FE 2 flag	FE 3 flag

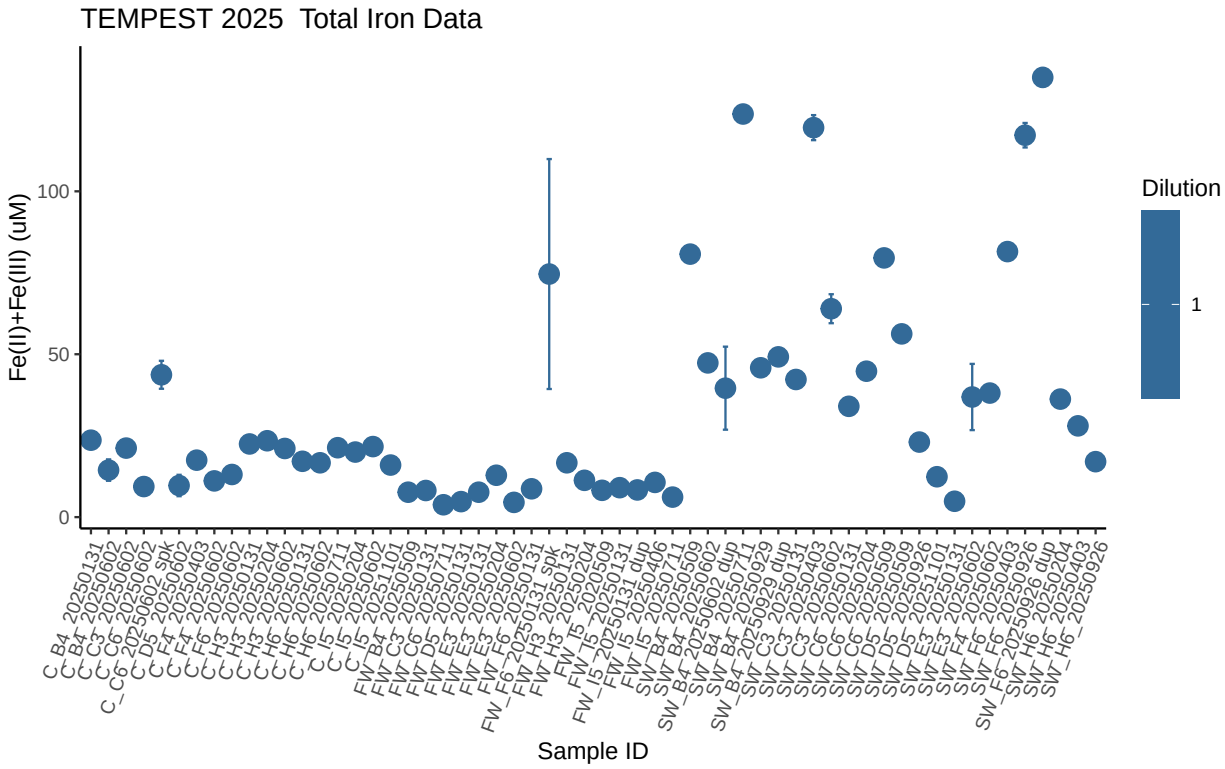
Table 5: Samples Below the Detection Limit that should be rerun at a lower dilution

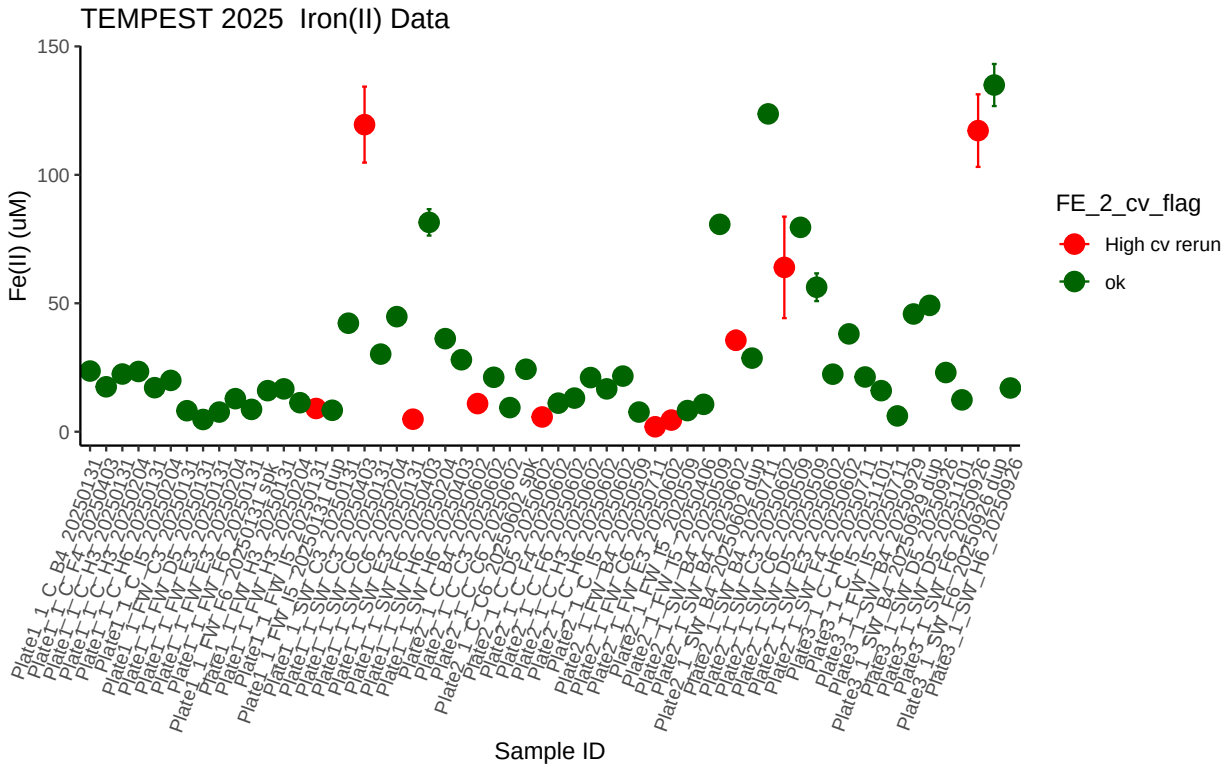
ID full	FE 2 mean	FE 3 mean	FE tot mean	FE 2 flag	FE 3 flag

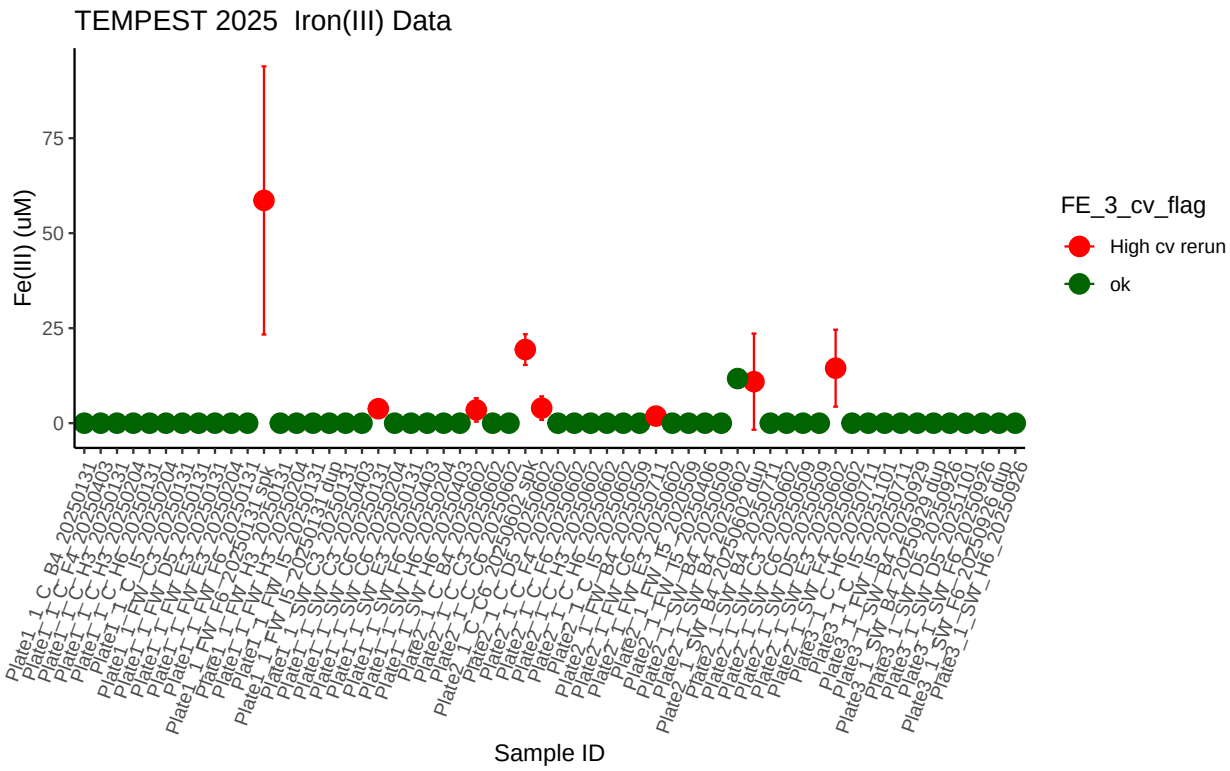
Plot data after bad reps were removed



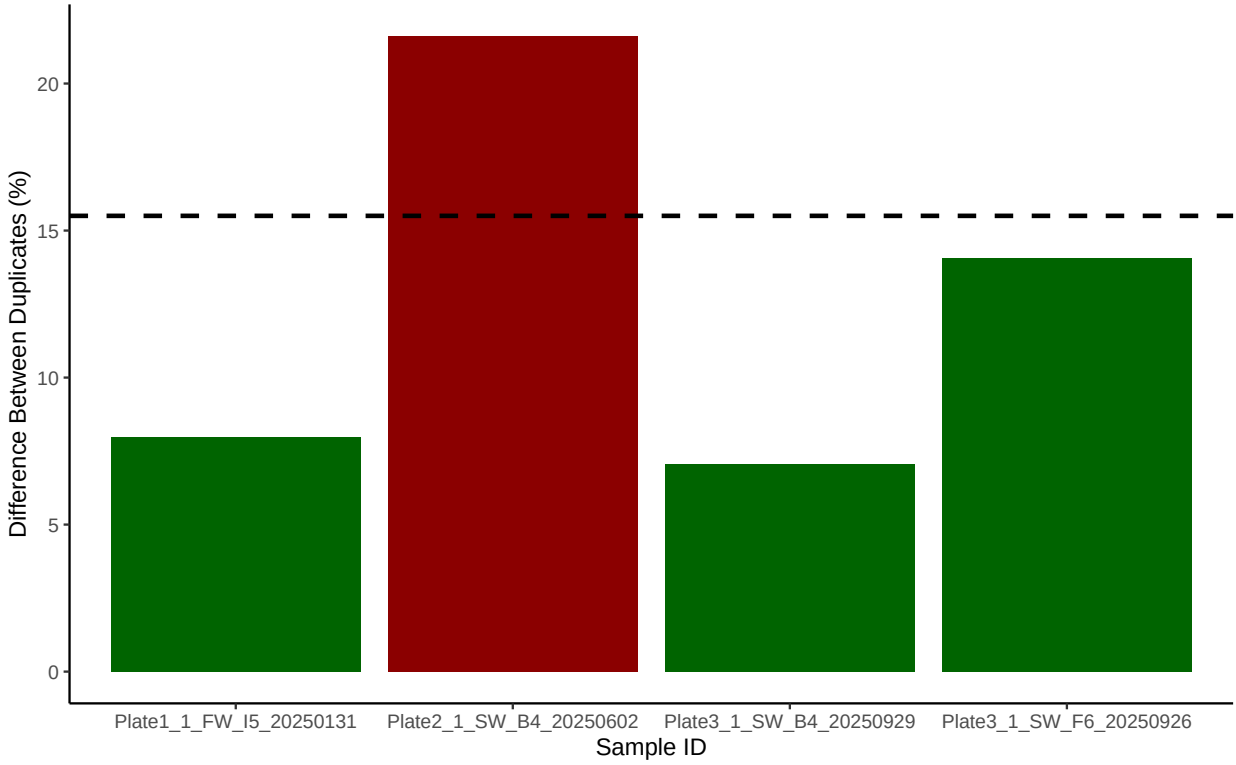


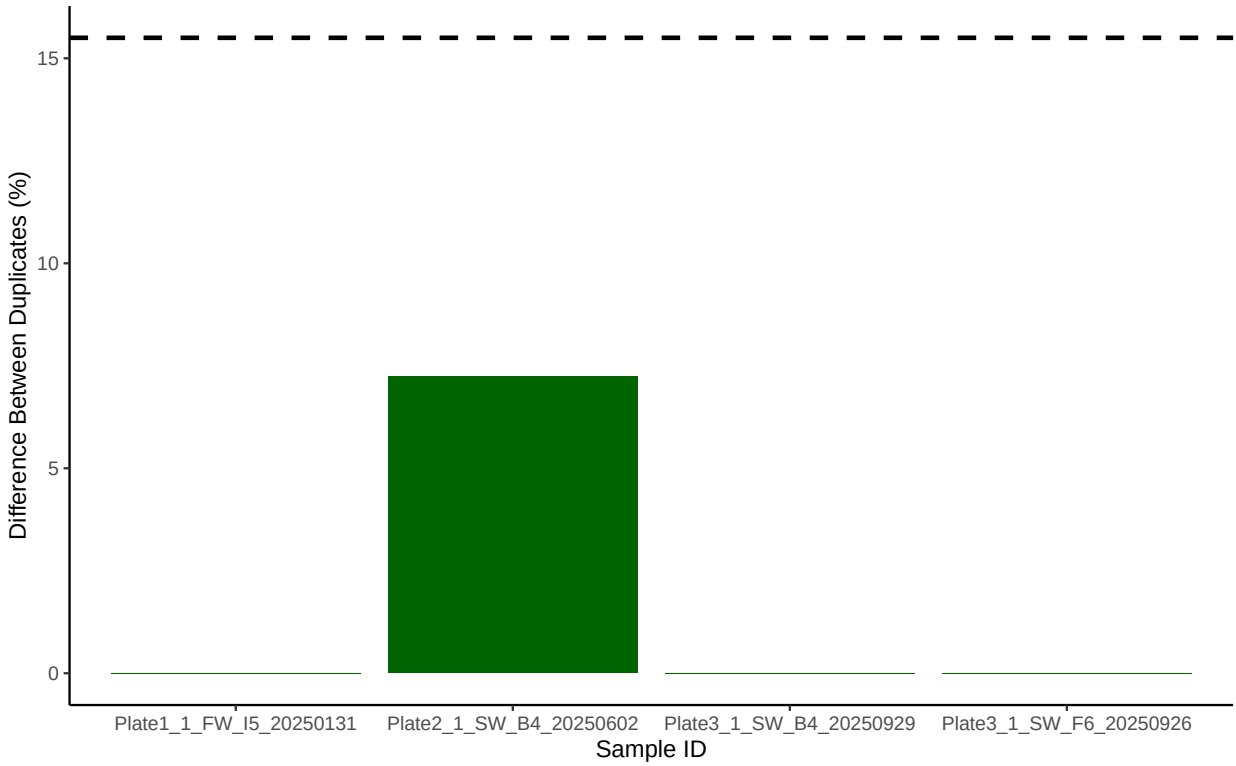

TEMPEST 2025 Total Iron Data
Fe(II)+Fe(III) (uM)
0
50
100
Sample ID
Dilution
1

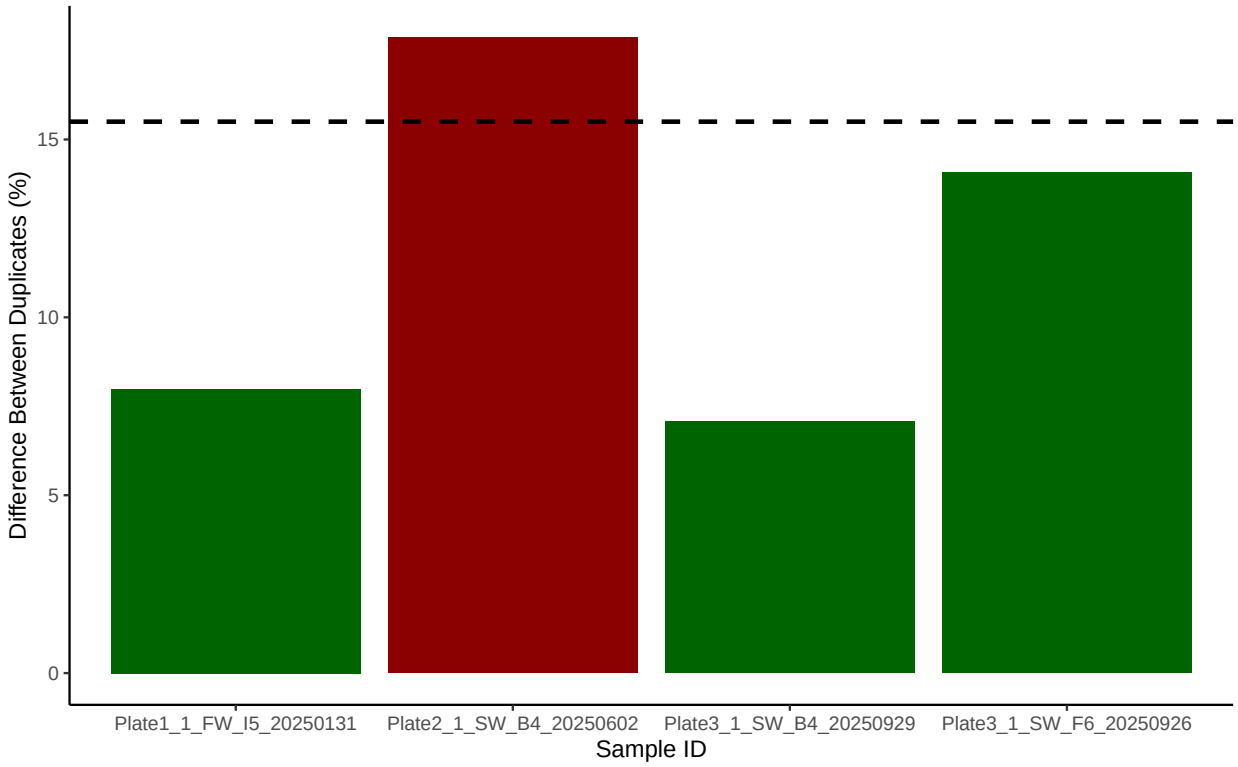

TEMPEST 2025 Iron(II) Data
Fe(II) (uM)
0
50
100
150
Sample ID
FE_2_cv_flag
High cv rerun
ok


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

Check Dups for QAQC



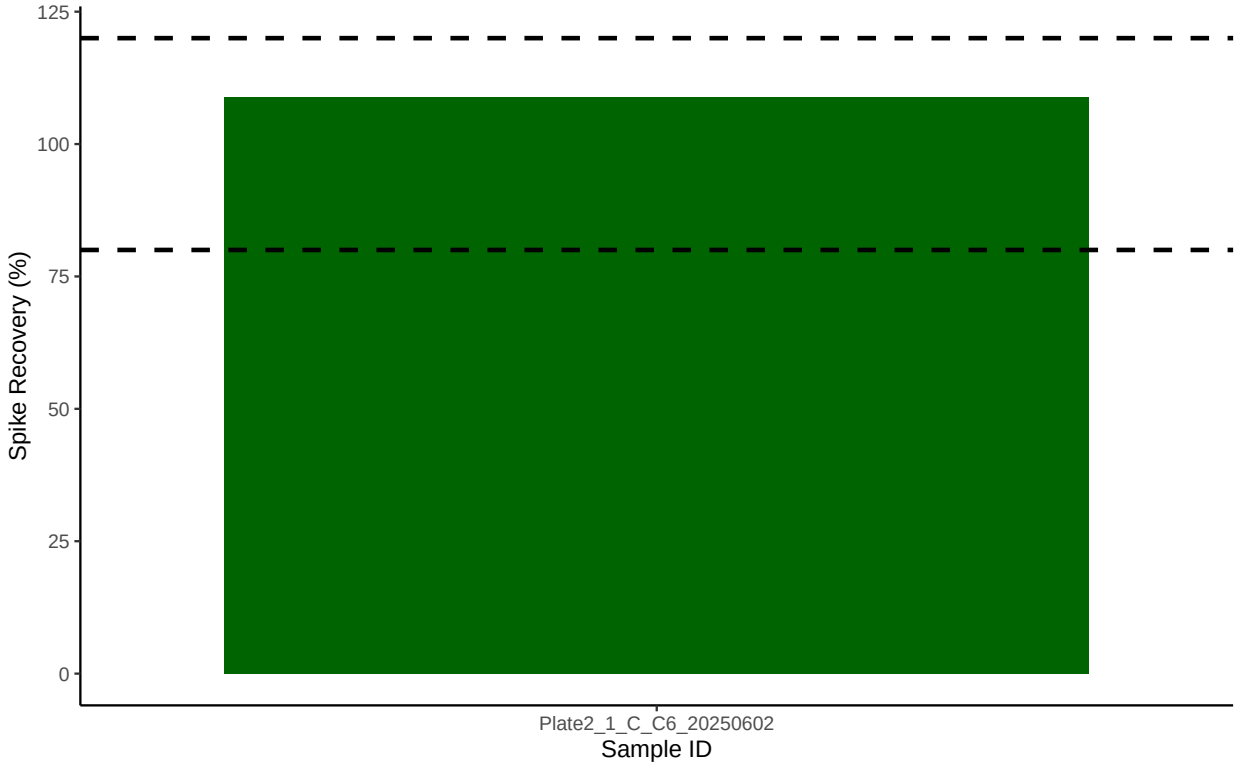





```
## [1] ">60% of Fe 2 Duplicates are within <10%"
```

```
## [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