PLS Network Comparison

10/27

0) Before processing

1. Copy file from Box
2. Do manual removal of 2nd column in LibreOffice
3. Compare

```
(base) laurenbell@10-248-131-65 Desktop % python checker.py -f PLS_CARLONI_L.csv "PLS_CARLONI copy.csv"
(base) laurenbell@10-248-131-65 Desktop %
```

1) QC

1) Filter out marked metabolites in QC file
2) Another issue here: I still had the old QC file, hadn’t removed 76

```
(base) laurenbell@10-248-131-65 Desktop % python checker.py -f pls_filtered_L.csv pls_filtered_A.csv
(base) laurenbell@10-248-131-65 Desktop %
```

2) Filter for CTRLs

1) filter out controls

```
(base) laurenbell@10-248-131-65 Desktop % python checker.py -f pls_DSS_CTRL_filtered_L.csv pls_DSS_CTRL_filtered_A.csv
(base) laurenbell@10-248-131-65 Desktop % python checker.py -f pls_LPS_CTRL_filtered_L.csv pls_LPS_CTRL_filtered_A.csv
(base) laurenbell@10-248-131-65 Desktop % python checker.py -f pls_VECPAC_CTRL_filtered_L.csv pls_VECPAC_CTRL_filtered_A.csv
(base) laurenbell@10-248-131-65 Desktop %
```

3) Log Transformation, Quantile Norm, 0 -> NaNs

1) Log2 transform data
2) Apply quantile normalization
3) Replace 0's in log transformed data to NaNs

```
(base) laurenbell@10-248-131-65 Desktop % python checker.py -f pls_DSS_CTRL_normalized_A.csv pls_DSS_post_norm.csv
(base) laurenbell@10-248-131-65 Desktop % python checker.py -f pls_LPS_CTRL_normalized_A.csv pls_LPS_post_norm.csv
(base) laurenbell@10-248-131-65 Desktop % python checker.py -f pls_VECPAC_CTRL_normalized_A.csv pls_VECPAC_post_norm.csv
(base) laurenbell@10-248-131-65 Desktop %
```

4) Metabolite Pairs

1) Compute correlations between each metabolite pair
2) Repeat for each model
3) Save p-value, correlation coefficient, and the number of samples
4) Used LibreOffice to change headers to match

```
(base) laurenbell@10-248-131-65 Desktop % python checker.py -f COMBINATIONS_pls_DSS_A.csv COMBINATIONS_pls_DSS_L.csv
(base) laurenbell@10-248-131-65 Desktop % python checker.py -f COMBINATIONS_pls_LPS_A.csv COMBINATIONS_pls_LPS_L.csv
(base) laurenbell@10-248-131-65 Desktop % python checker.py -f COMBINATIONS_pls_VECPAC_A.csv COMBINATIONS_pls_VECPAC_L.csv
(base) laurenbell@10-248-131-65 Desktop %
```

5) FDR and Meta-analysis Table

1) Change code to match headers
2) Using metacor(), compute meta-analysis correlation coefficients and FDR values

```
(base) laurenbell@10-248-131-65 Desktop % python checker.py -f "Meta-analysis + FDR Table.csv" quantile_fdr_table_10_27.csv
(base) laurenbell@10-248-131-65 Desktop %
```

7) Network Properties Table

1) calculate network properties

```
(base) laurenbell@10-248-131-65 Desktop % python checker.py -f quantile_network_properties_L.csv quantile_network_properties_A.csv
(base) laurenbell@10-248-131-65 Desktop %
```