

RedShift AQS³ delta Analytics Results

Report Date: Friday, May 5, 2023 9:11:10 AM
 Report File: "AnalysisReport_20230505_071110Z.pdf"
 Username: Default UserEx
 Version(s): GUI: 2.5.98.4131
 DataSet Name: "20221122_Uni_Graz"
 Proc. Data Folder: "pdata_Evaluation report_20221124_114232Z"
 Processed Date: Thursday, November 24, 2022 12:42:32 PM

Table of Analyzed Sample Data:





| Clr | Included? | Collection Type | Replicate | Sample Name |
|---|-----------|--------------------|-----------|---------------|
|  | Yes | Sample/Buffer (SB) | (avg) | RS_1.Buffer 1 |
|  | Yes | Sample/Buffer (SB) | (avg) | RS_2.Buffer 2 |
|  | Yes | Sample/Buffer (SB) | (avg) | RS_3.Buffer 3 |
|  | Yes | Model Protein | | NIST mAb |

Table of Sample Replicates in Averaging:










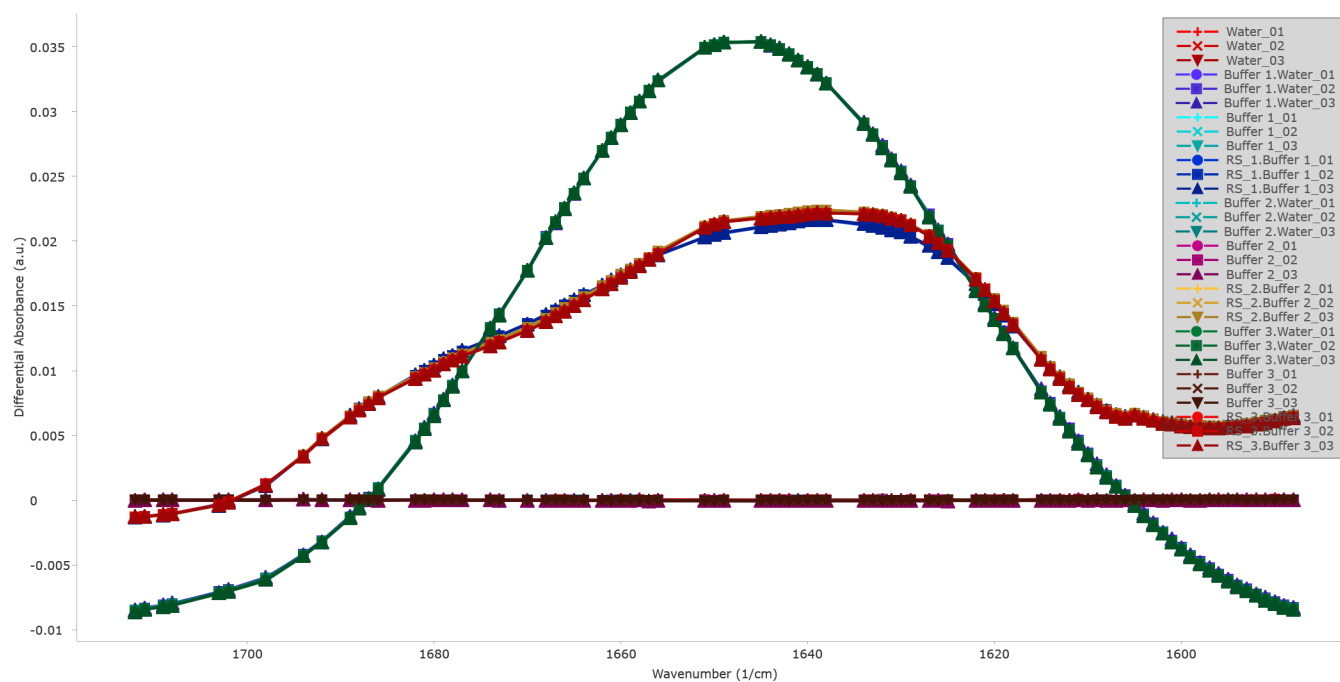
| Clr | Included? | Collection Type | Replicate | Sample Name |
|---|-----------|--------------------|-----------|---------------|
|  | Yes | Sample/Buffer (SB) | 01 | RS_1.Buffer 1 |
|  | Yes | Sample/Buffer (SB) | 02 | RS_1.Buffer 1 |
|  | Yes | Sample/Buffer (SB) | 03 | RS_1.Buffer 1 |
|  | Yes | Sample/Buffer (SB) | 01 | RS_2.Buffer 2 |
|  | Yes | Sample/Buffer (SB) | 02 | RS_2.Buffer 2 |
|  | Yes | Sample/Buffer (SB) | 03 | RS_2.Buffer 2 |
|  | Yes | Sample/Buffer (SB) | 01 | RS_3.Buffer 3 |
|  | Yes | Sample/Buffer (SB) | 02 | RS_3.Buffer 3 |
|  | Yes | Sample/Buffer (SB) | 03 | RS_3.Buffer 3 |

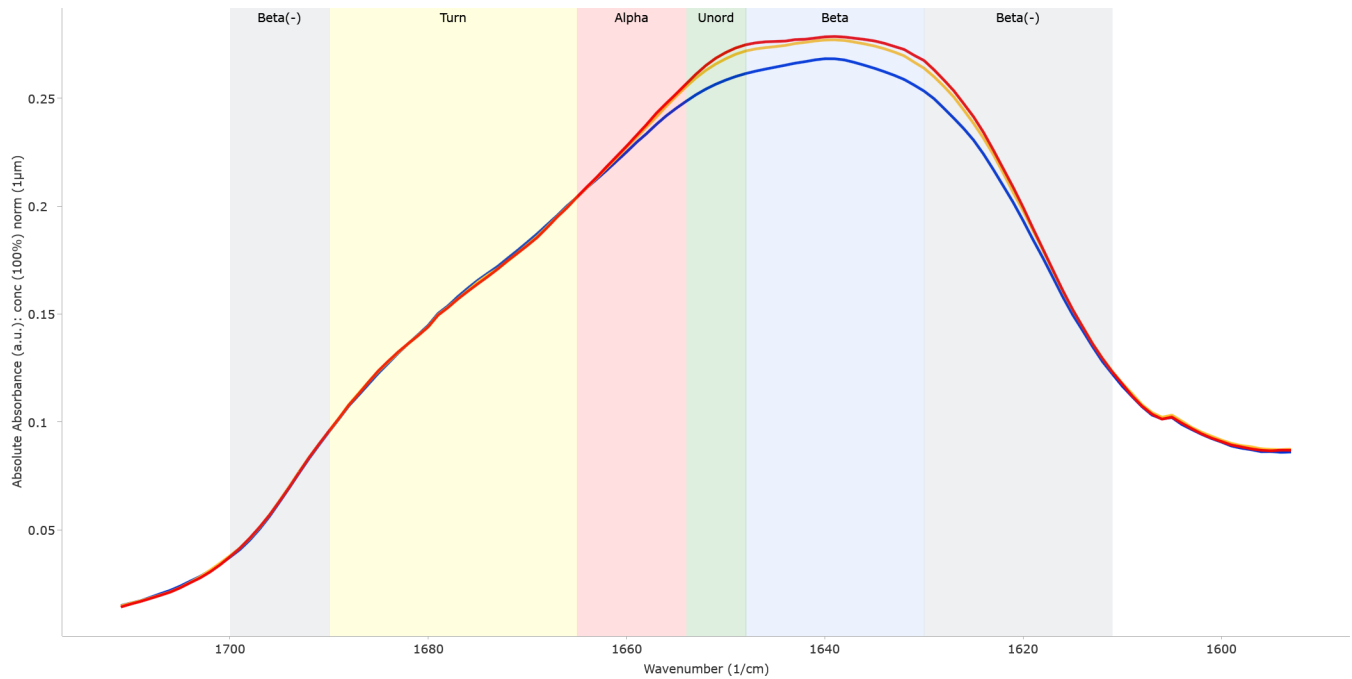
Table of Water and Buffer Replicates:

| Included? | Collection Type | Replicate | Sample Name |
|-----------|--------------------|-----------|----------------|
| Yes | Water/Water (WW) | 01 | Water |
| Yes | Water/Water (WW) | 02 | Water |
| Yes | Water/Water (WW) | 03 | Water |
| Yes | Buffer/Water (BW) | 01 | Buffer 1.Water |
| Yes | Buffer/Water (BW) | 02 | Buffer 1.Water |
| Yes | Buffer/Water (BW) | 03 | Buffer 1.Water |
| Yes | Buffer/Buffer (BB) | 01 | Buffer 1 |
| Yes | Buffer/Buffer (BB) | 02 | Buffer 1 |
| Yes | Buffer/Buffer (BB) | 03 | Buffer 1 |
| Yes | Buffer/Water (BW) | 01 | Buffer 2.Water |
| Yes | Buffer/Water (BW) | 02 | Buffer 2.Water |
| Yes | Buffer/Water (BW) | 03 | Buffer 2.Water |
| Yes | Buffer/Buffer (BB) | 01 | Buffer 2 |
| Yes | Buffer/Buffer (BB) | 02 | Buffer 2 |
| Yes | Buffer/Buffer (BB) | 03 | Buffer 2 |
| Yes | Buffer/Water (BW) | 01 | Buffer 3.Water |
| Yes | Buffer/Water (BW) | 02 | Buffer 3.Water |
| Yes | Buffer/Water (BW) | 03 | Buffer 3.Water |
| Yes | Buffer/Buffer (BB) | 01 | Buffer 3 |
| Yes | Buffer/Buffer (BB) | 02 | Buffer 3 |
| Yes | Buffer/Buffer (BB) | 03 | Buffer 3 |

Graph Results: Raw Diff AU



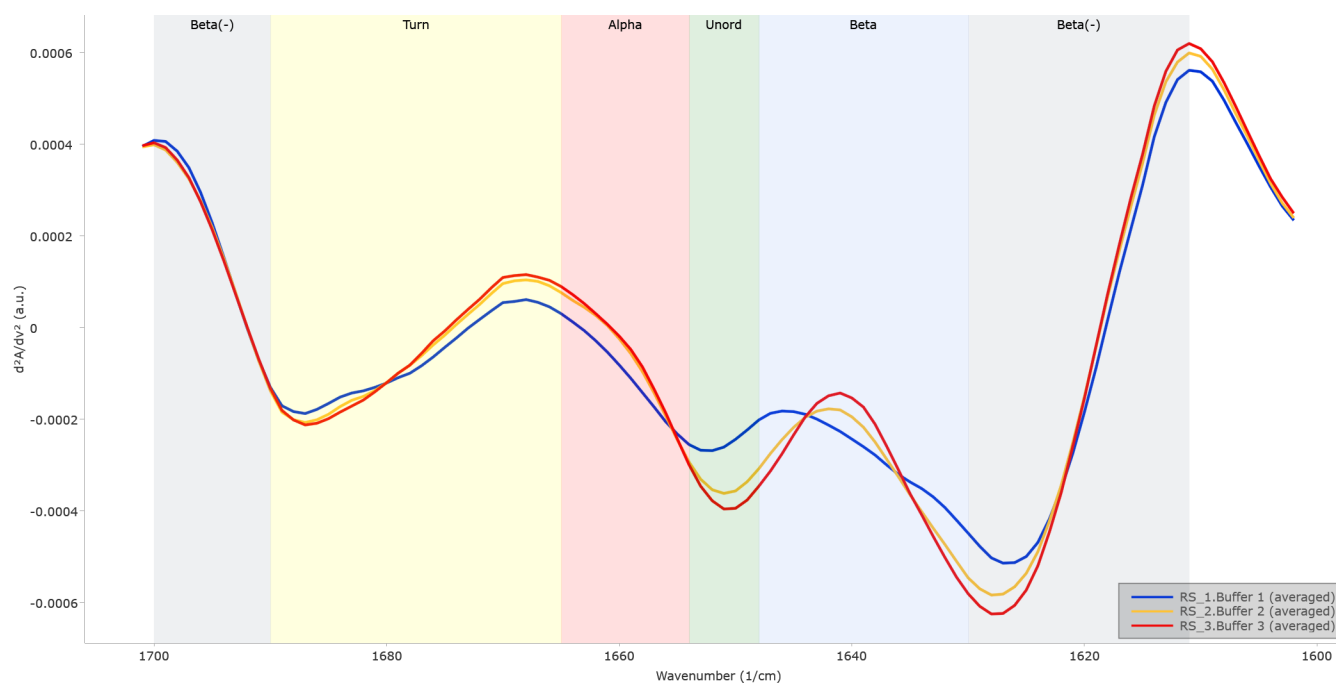
Graph Results: Absolute AU



Analysis Settings for Absolute Spectrum:

Cell Pathlength(μm): 23.50
Water Data: "water spectra"
Normalization
100% Conc: True
1 μm Path: True
Spacing(1/cm): 1.0
Interpolation: Spline

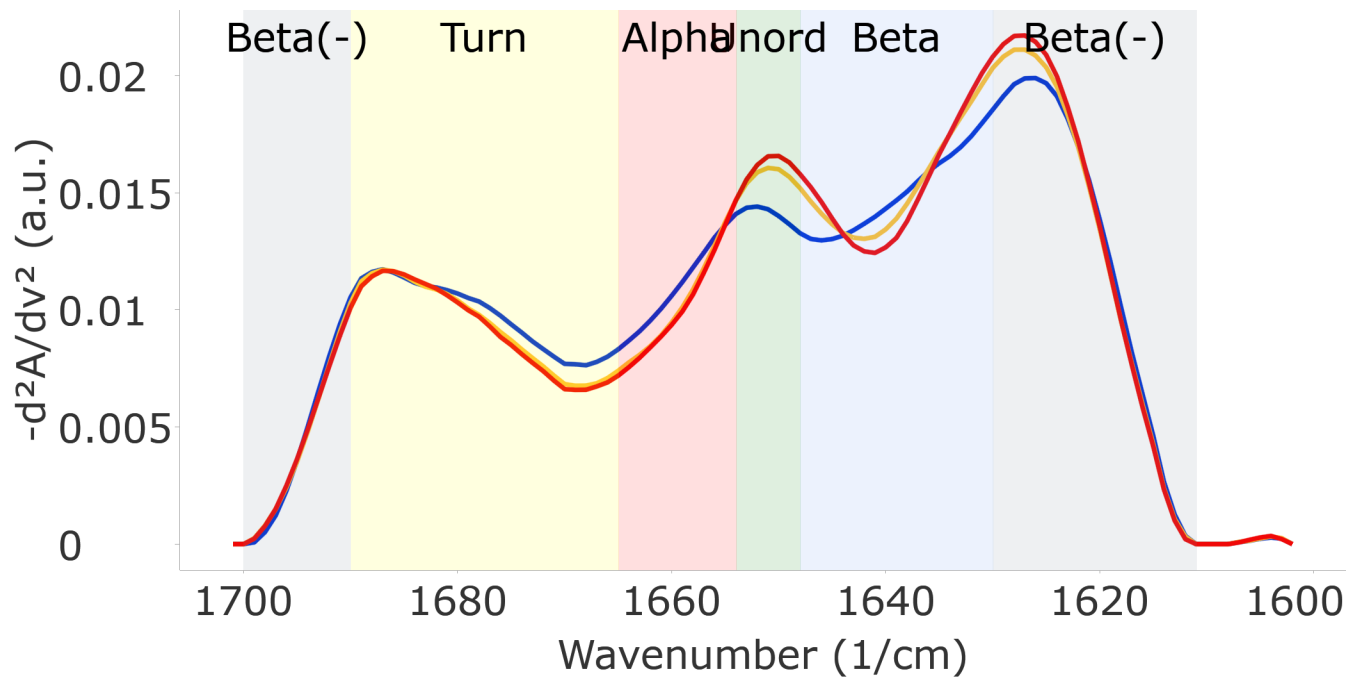
Graph Results: Second Derivative



Analysis Settings for Second Derivative:

Normalization: False
Smoothing Window Size
Sample/Model: 19

Graph Results: Similarity (Area of Overlap)



Analysis Settings for Similarity (Area of Overlap):

| | |
|------------------------|-------------------|
| Spectral Range: | Full Data Range |
| Baseline: | Rubberband |
| Normalization: | Normalize to Area |
| Comparison: | Mean/Selected |
| Include Model Protein: | False |

Graph of Area of Overlap and Comparison Set:

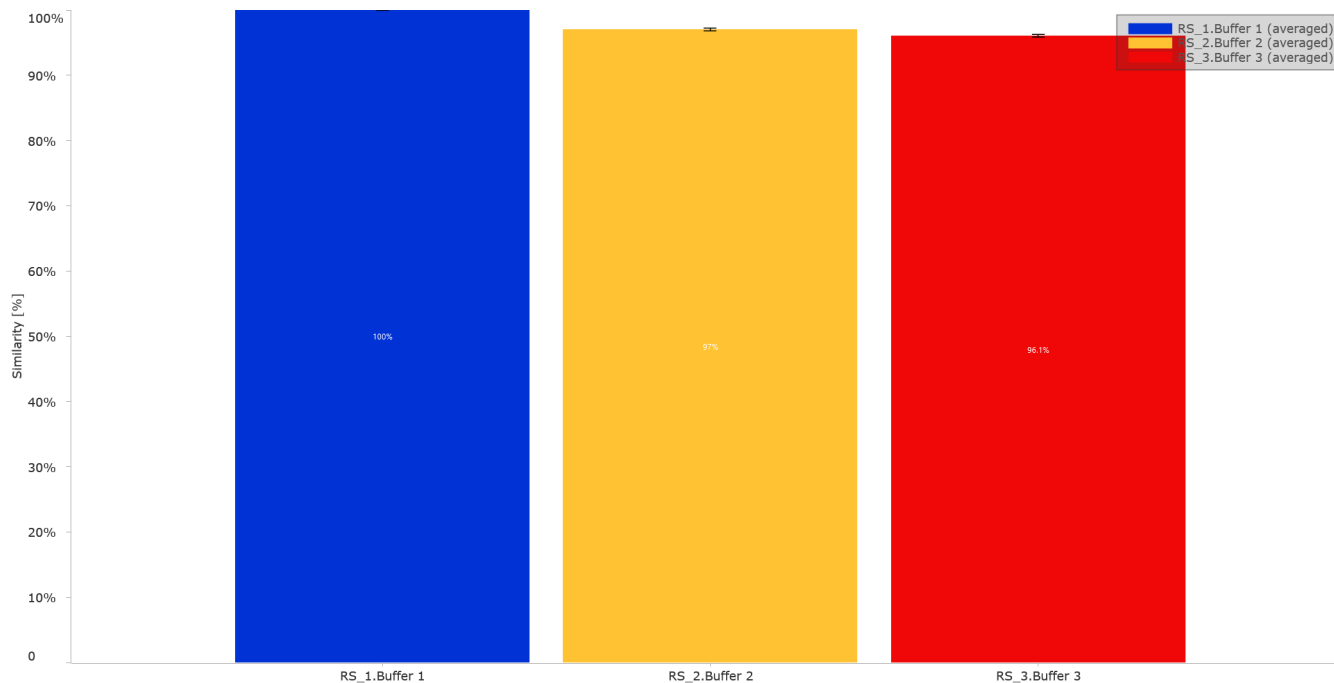


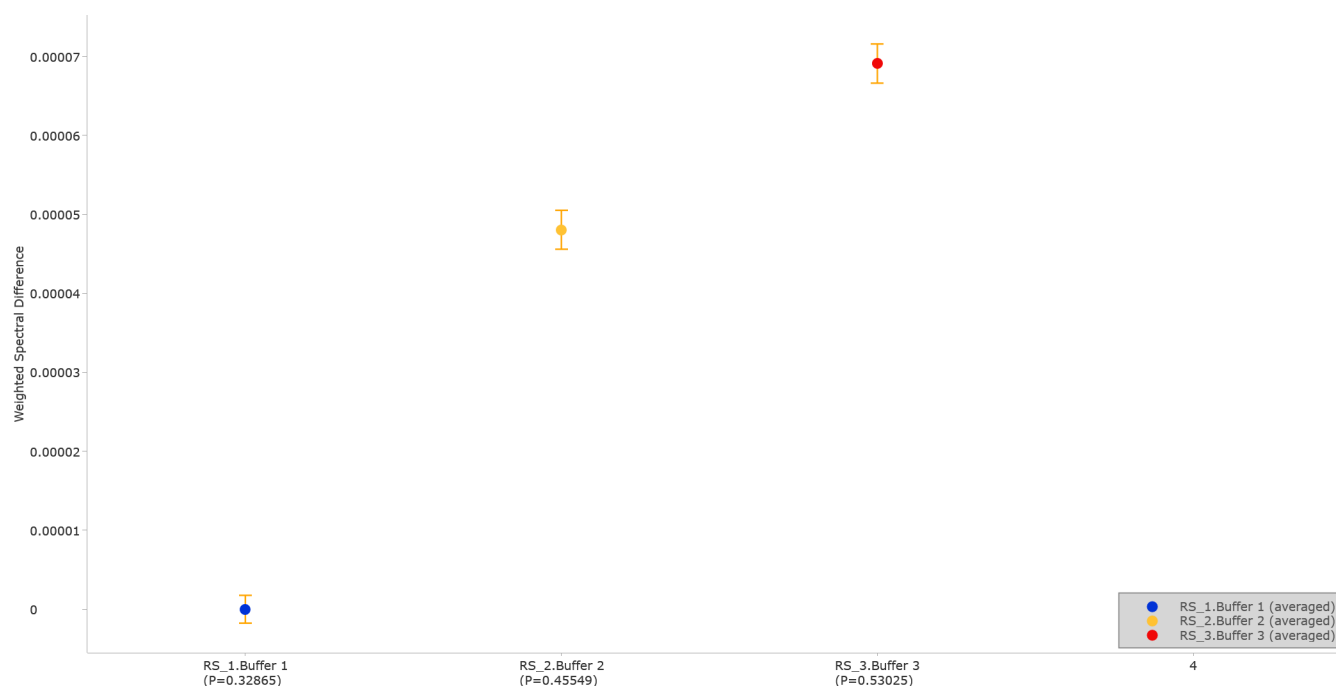
Table of Area of Overlap and Comparison Set:

| AO(%) | CompareSet | Replicate | Sample Name |
|-------|------------|-----------|---------------|
| 100.0 | Yes | (avg) | RS_1.Buffer 1 |
| 97.0 | No | (avg) | RS_2.Buffer 2 |
| 96.1 | No | (avg) | RS_3.Buffer 3 |
| 72.5 | No | | NIST mAb |

Similarity (Area of Overlap) Replicate Summary Table:

| Conc (mg/mL) | Mean±SD | Repeat. | AO (%) of Replicates | Sample Name |
|--------------|------------|---------|----------------------|---------------|
| 5.00 | 99.72±0.04 | 99.72 | 99.8, 99.7, 99.7 | RS_1.Buffer 1 |
| 5.00 | 96.92±0.21 | 99.54 | 96.7, 97.0, 97.1 | RS_2.Buffer 2 |
| 5.00 | 96.02±0.20 | 99.56 | 95.9, 95.9, 96.2 | RS_3.Buffer 3 |

Graph Results: Similarity (Weighted Spectral Difference)



Analysis Settings for Similarity (Weighted Spectral Difference):

Data Used: 2nd Derivative
 Comparison: Mean/Selected

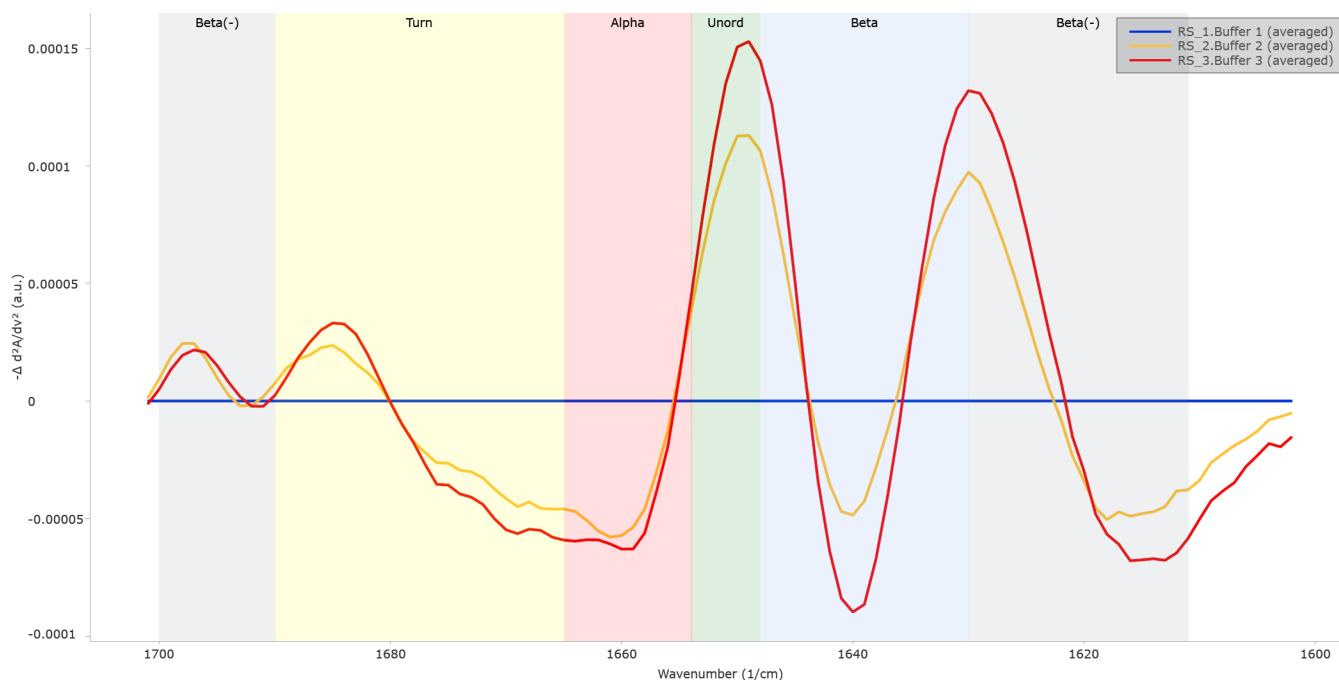
Table of Weighted Spectral Difference and Comparison Set:

| WSD | CompareSet | Replicate | Sample Name |
|------------|------------|-----------|---------------|
| 0 | Yes | (avg) | RS_1.Buffer 1 |
| 4.805e-05 | No | (avg) | RS_2.Buffer 2 |
| 6.9098e-05 | No | (avg) | RS_3.Buffer 3 |
| 0.00052173 | No | | NIST mAb |

Area of Overlap and Weighted Spectral Difference Summary Table

| Sample | AO Compare Set? | AO(%) | WSD Compare Set? | WSD | P Value |
|---------------------|-----------------|-------|------------------|------------|---------|
| RS_1.Buffer 1_(avg) | Yes | 100.0 | Yes | 0 | 0.32865 |
| RS_3.Buffer 3_(avg) | No | 96.1 | No | 6.9098e-05 | 0.53025 |
| RS_2.Buffer 2_(avg) | No | 97.0 | No | 4.805e-05 | 0.45549 |
| NIST mAb | No | 72.5 | No | 0.00052173 | N/A |

Graph Results: Delta



Analysis Settings for Delta:

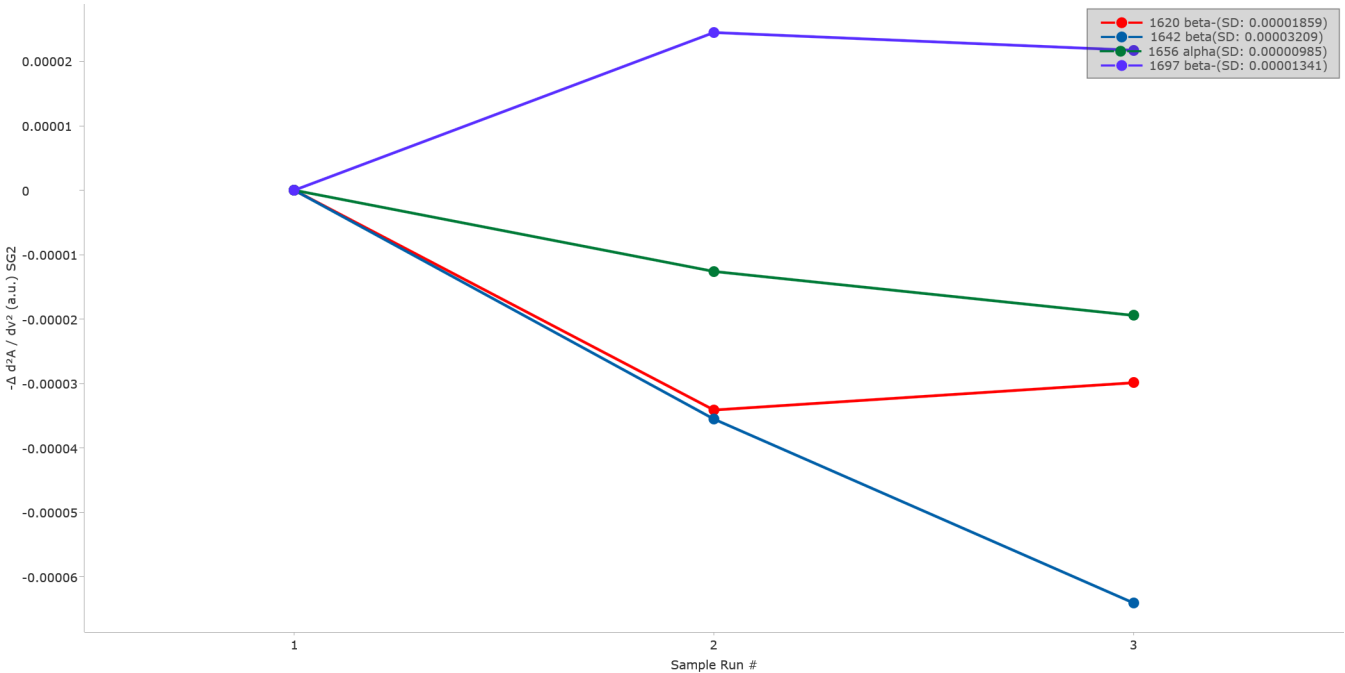
Use 2ndDeriv: True
 Comparison: Mean/Selected
 Include Model Protein: False
 Min/Max Delta Range: 0.0000000E+000 to 0.0000000E+000

Table of Delta Bounds and Comparison Set:

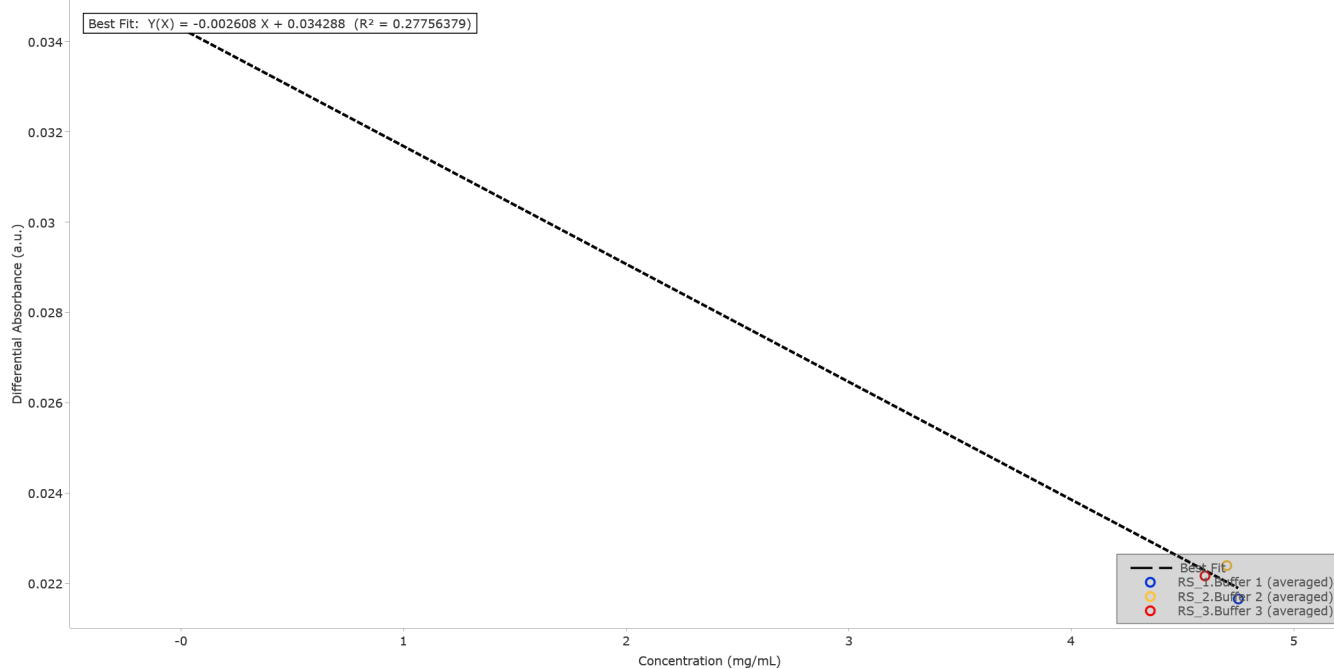
| Within Min/Max Bounds | CompareSet | Replicate | Sample Name |
|-----------------------|------------|-----------|---------------|
| N/A | Yes | (avg) | RS_1.Buffer 1 |
| N/A | No | (avg) | RS_2.Buffer 2 |
| N/A | No | (avg) | RS_3.Buffer 3 |
| N/A | No | | NIST mAb |

Graph Results: Stability

Data used for Stability: Delta



Graph Results: Quantitation



Analysis Settings for Quantitation:

Model Protein: NIST mAb
 Concentration Plotted: Fit

Table of Concentrations and Displacement Factors:

| Conc (mg/mL) | Fit Conc(mg/mL) | Fit DF | Replicate | Sample Name |
|--------------|-----------------|--------|-----------|---------------|
| 5.00 | 4.75 | 0.6000 | (avg) | RS_1.Buffer 1 |
| 5.00 | 4.70 | 0.6000 | (avg) | RS_2.Buffer 2 |
| 5.00 | 4.60 | 0.5940 | (avg) | RS_3.Buffer 3 |

Graph Results: Gaussian Fit



Table of Gaussian Fit R²:

| Gaussian Fit R² Value | Replicate | Sample Name |
|-----------------------|-----------|---------------|
| 0.99964 | (avg) | RS_1.Buffer 1 |
| 0.99967 | (avg) | RS_2.Buffer 2 |
| 0.99969 | (avg) | RS_3.Buffer 3 |

Table of Gaussian Term Settings (*default):

| Wavelength(1/cm) | Structure | PeakWindow(+/-) | FWHM(1/cm) |
|------------------|-----------|-----------------|------------|
| 1597.0 | side | 1.0 * | 10 * |
| 1610.0 | beta- | -5.0 to 0.0 * | 6 * |
| 1618.0 | beta- | 3.0 * | 6 * |
| 1626.0 | beta- | 1.0 * | 6 * |
| 1632.0 | beta | 1.0 * | 6 * |
| 1642.0 | beta | 1.0 * | 6 * |
| 1650.0 | unord | 1.0 * | 6 * |
| 1656.0 | alpha | 1.0 * | 6 * |
| 1660.0 | turn | 1.0 * | 6 * |
| 1666.0 | turn | 1.0 * | 6 * |
| 1672.0 | turn | 1.0 * | 6 * |
| 1680.0 | turn | 1.0 * | 6 * |
| 1688.0 | turn | 1.0 * | 6 * |
| 1690.0 | beta | 1.0 * | 6 * |
| 1695.0 | beta- | 1.0 * | 6 * |
| 1704.0 | side | 1.0 * | 20 * |

Graph Results: HOS (Structure)

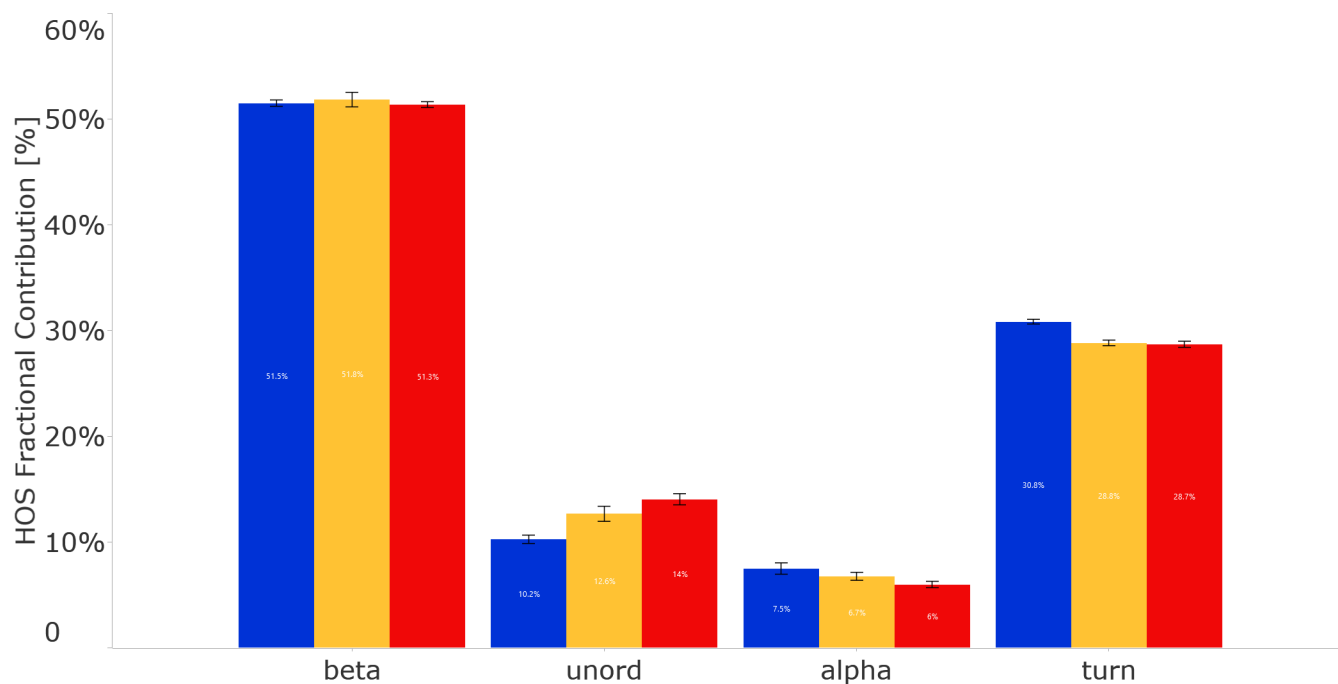


Table of HOS Statistics:

| HOS Bin Name | Fractional(%) Mean | Fractional(%) StdDev |
|--------------|--------------------|----------------------|
| beta | 51.5 | 0.24 |
| unord | 12.3 | 1.92 |
| alpha | 6.7 | 0.75 |
| turn | 29.4 | 1.20 |

High Order Structure (HOS) Replicate Summary Table:

| Conc (mg/mL) | beta Mean±SD | unord Mean±SD | alpha Mean±SD | turn Mean±SD | Sample Name |
|--------------|-----------------|------------------|------------------|-----------------|---------------|
| 5.00 | 51.7±0.30 | 10.2±0.40 | 7.4±0.54 | 30.7±0.22 | RS_1.Buffer 1 |
| 5.00 | 52.0±0.69 | 12.4±0.71 | 6.7±0.38 | 28.9±0.26 | RS_2.Buffer 2 |
| 5.00 | 51.6±0.27 | 13.9±0.53 | 5.9±0.30 | 28.6±0.29 | RS_3.Buffer 3 |