

## Spectral Analysis Report



Analysis performed on: 2025-07-07 13:17:25

*Generated by MetaspeQ Spectral Intelligence Engine*

# Model Summary

Best Model: RandomFrog\_SNV\_RF\_Full

RMSE: 20.4817

R<sup>2</sup>: 0.9675

Q<sup>2</sup>: -0.1739

Latent Variables: N/A

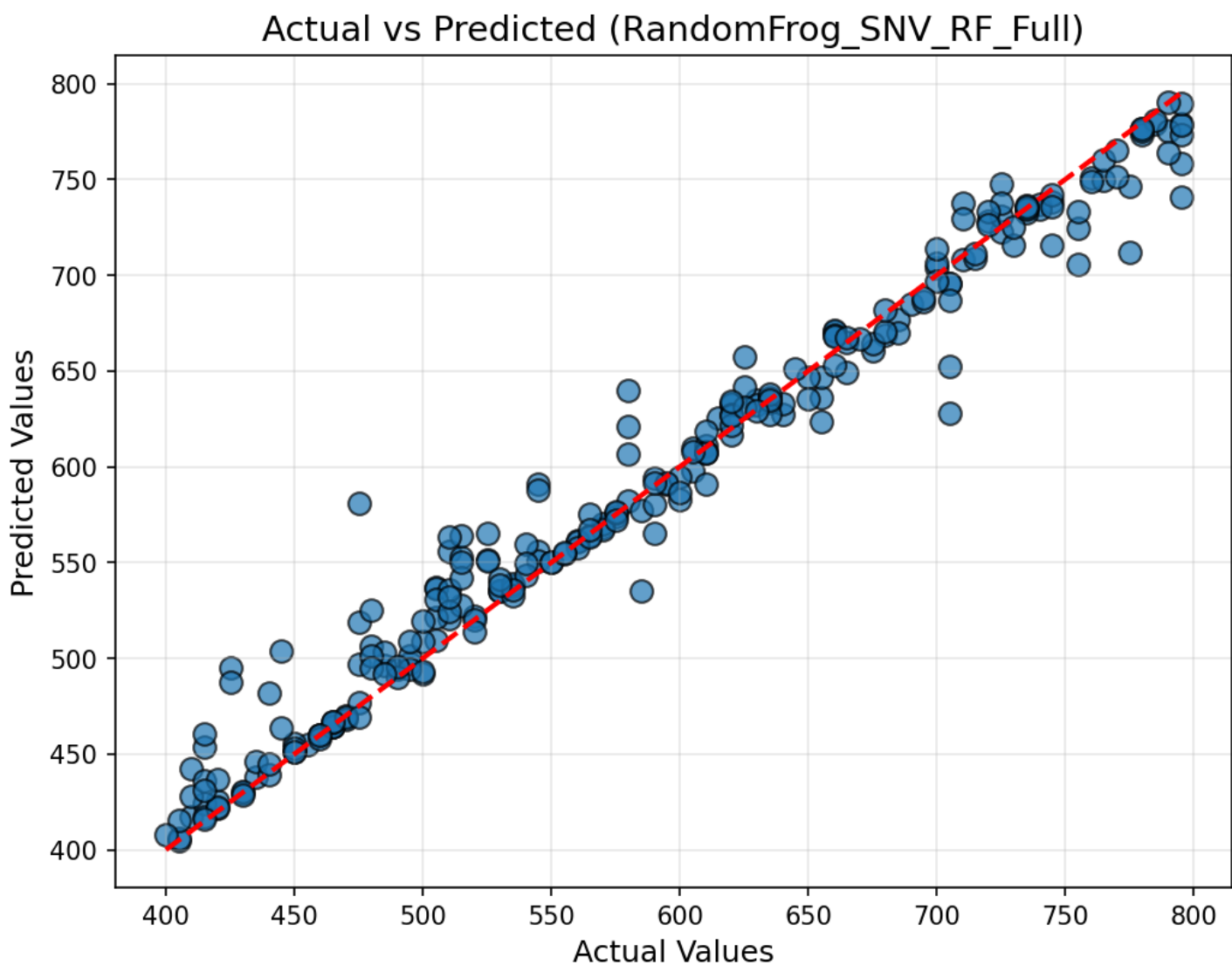
Feature Selection: RandomFrog

Number of Selected Wavelengths: 102

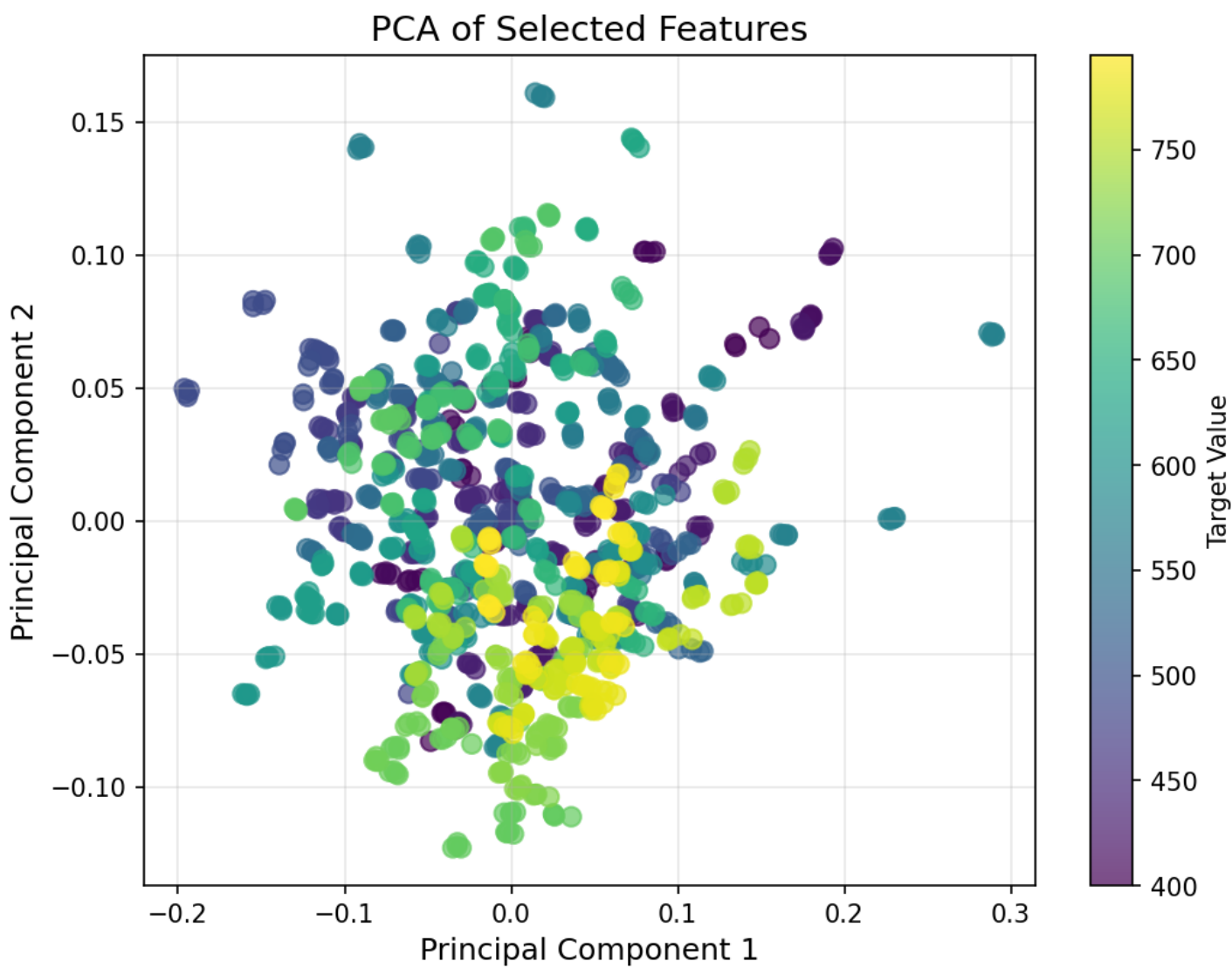
# Selected Wavelengths

896.16 nm	899.88 nm	918.43 nm	925.82 nm	933.20 nm
936.89 nm	966.23 nm	984.46 nm	1002.61 nm	1013.45 nm
1017.06 nm	1020.67 nm	1031.46 nm	1049.39 nm	1056.53 nm
1074.34 nm	1077.89 nm	1081.44 nm	1084.98 nm	1092.06 nm
1116.72 nm	1134.22 nm	1141.20 nm	1144.68 nm	1155.11 nm
1158.58 nm	1162.04 nm	1165.50 nm	1179.31 nm	1182.75 nm
1199.90 nm	1203.32 nm	1206.73 nm	1216.95 nm	1220.35 nm
1227.13 nm	1250.74 nm	1260.80 nm	1270.82 nm	1287.42 nm
1290.73 nm	1294.03 nm	1297.33 nm	1300.63 nm	1307.20 nm
1313.76 nm	1317.03 nm	1333.32 nm	1336.56 nm	1359.12 nm
1368.72 nm	1375.09 nm	1378.27 nm	1397.24 nm	1409.79 nm
1422.25 nm	1428.45 nm	1431.54 nm	1437.71 nm	1443.85 nm
1446.92 nm	1456.08 nm	1471.25 nm	1483.29 nm	1489.28 nm
1495.25 nm	1507.12 nm	1510.07 nm	1515.96 nm	1518.90 nm
1533.51 nm	1536.42 nm	1539.32 nm	1547.99 nm	1550.87 nm
1553.74 nm	1556.61 nm	1559.48 nm	1568.04 nm	1570.88 nm
1579.38 nm	1590.65 nm	1593.45 nm	1599.04 nm	1607.40 nm
1610.17 nm	1612.94 nm	1615.71 nm	1632.20 nm	1637.67 nm
1640.39 nm	1643.11 nm	1656.65 nm	1664.73 nm	1670.09 nm
1672.77 nm	1675.44 nm	1683.43 nm	1688.74 nm	1691.40 nm
1694.04 nm	1701.97 nm			

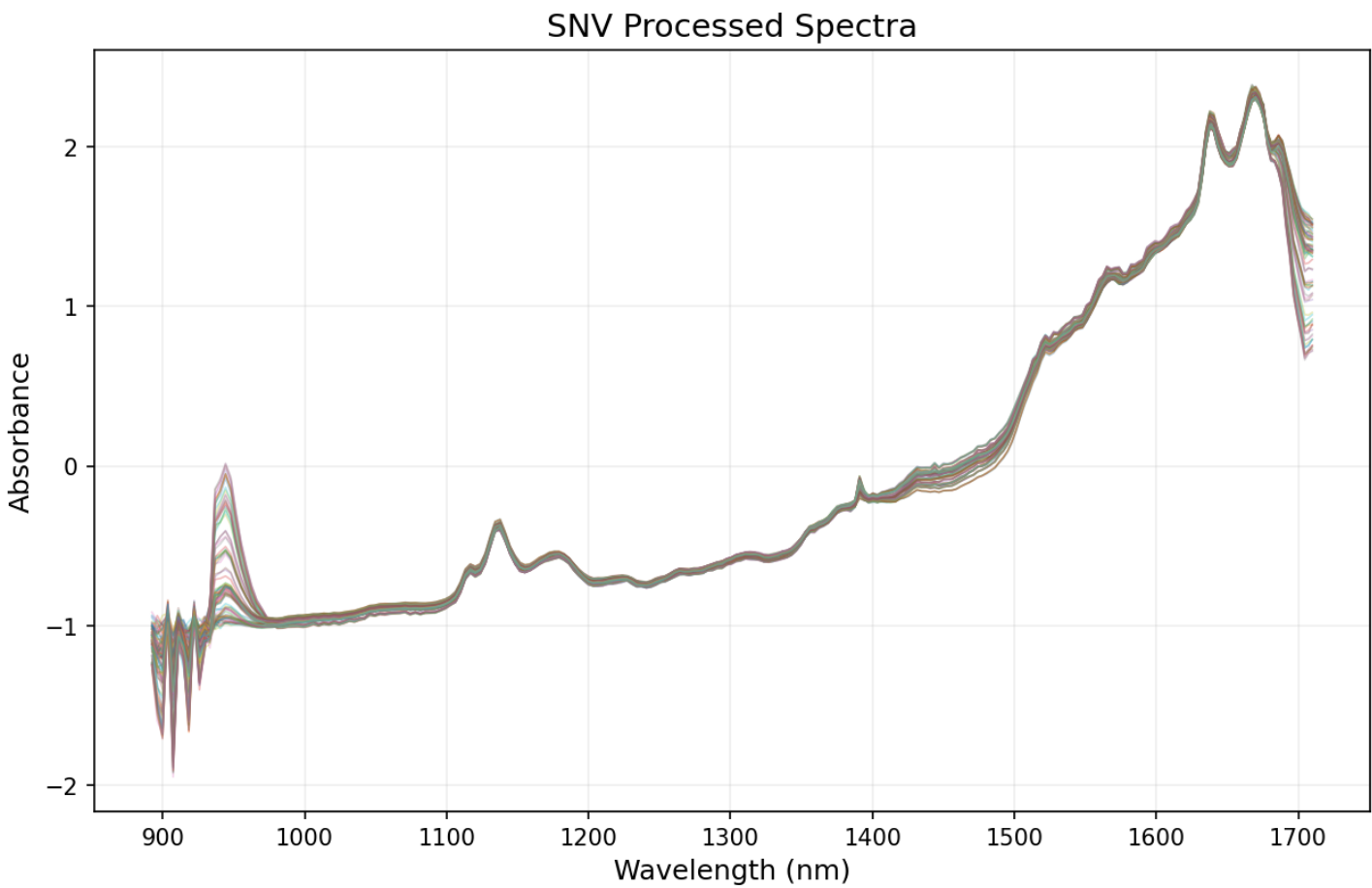
# Actual vs Predicted Values



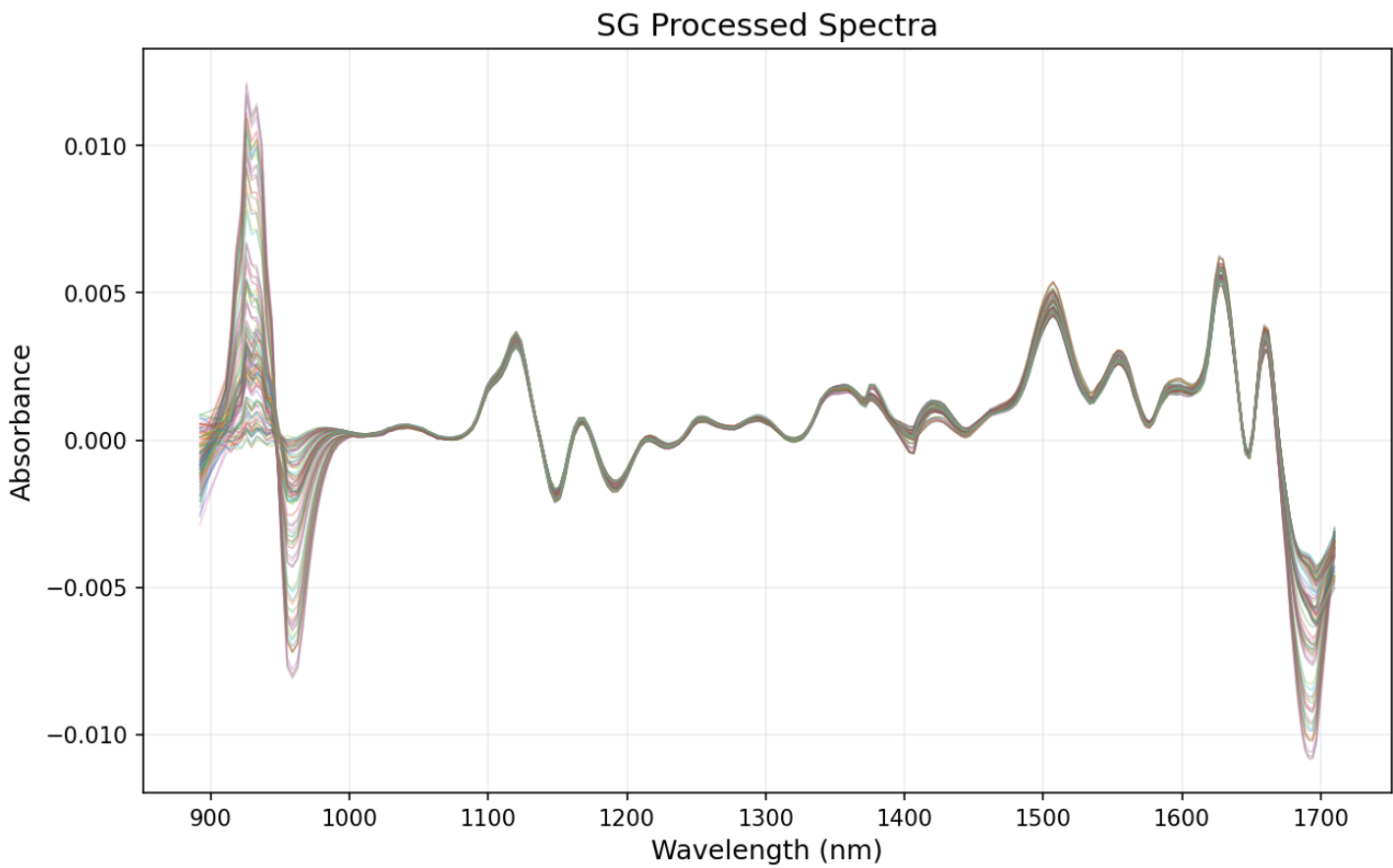
# PCA Visualization of Selected Features



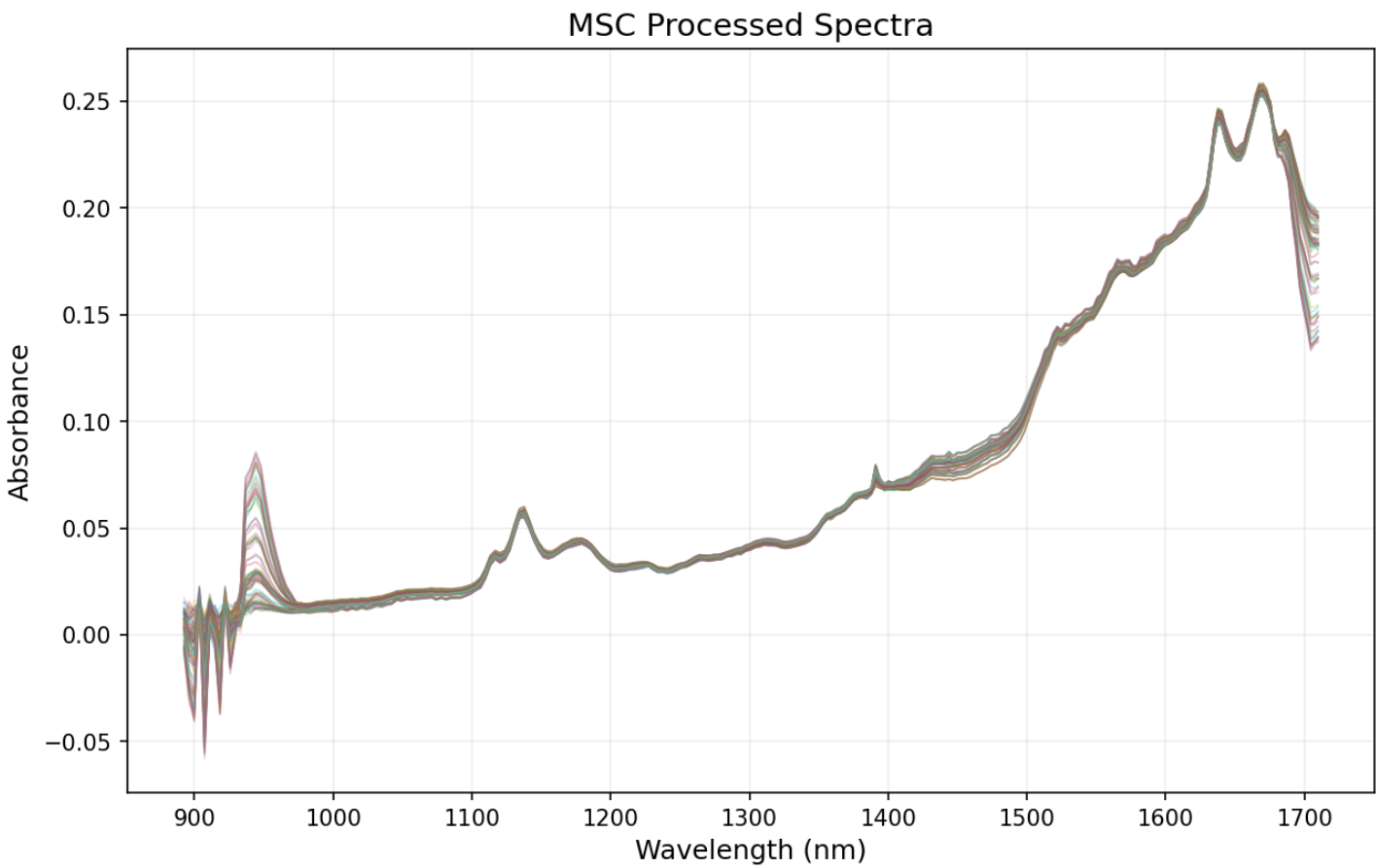
# Standard Normal Variate (SNV) Processed Spectra



# Savitzky-Golay Processed Spectra

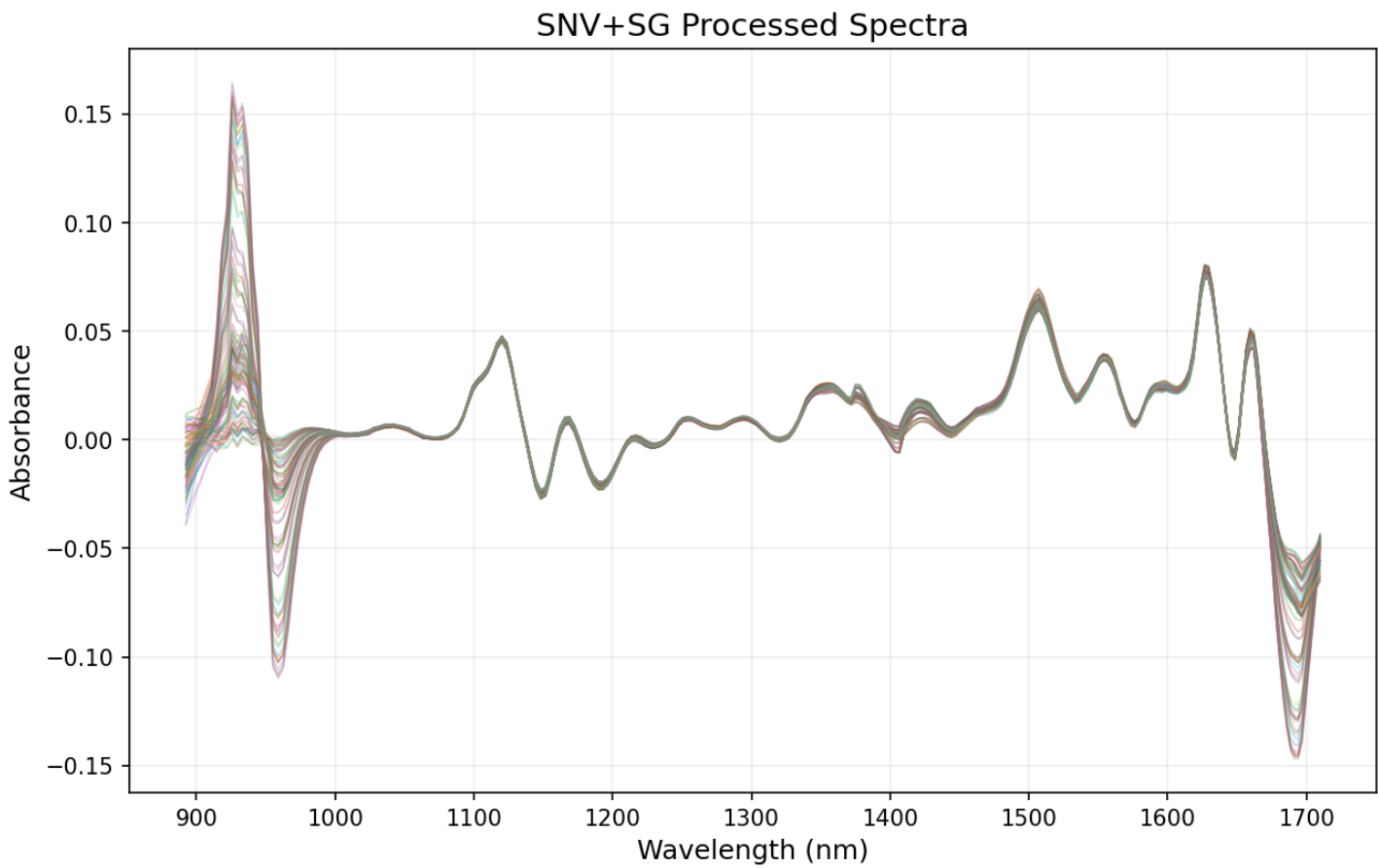


# Multiplicative Scatter Correction (MSC) Processed Spectra





# SNV + Savitzky-Golay Processed Spectra



# Model Evaluation Results

Feature	Process	Model	LatentVariables	Method	RMSE	R <sup>2</sup>	Q <sup>2</sup>
CARS	SNV	PLS	3	Full	87.705	0.404	-0.323
CARS	SNV	RF	NA	Full	23.637	0.957	-0.037
CARS	SNV	SVM	NA	Full	113.804	-0.003	-0.688
CARS	SNV	ANN	NA	Full	66.048	0.662	-0.286
CARS	SNV	PLS	1	PCA	105.433	0.139	-1.193
CARS	SNV	RF	NA	PCA	45.313	0.841	-0.540
CARS	SNV	SVM	NA	PCA	100.426	0.219	-0.656
CARS	SNV	ANN	NA	PCA	65.323	0.669	-0.728
CARS	SG	PLS	3	Full	83.758	0.457	-0.192
CARS	SG	RF	NA	Full	25.260	0.951	0.069
CARS	SG	SVM	NA	Full	112.320	0.023	-0.745
CARS	SG	ANN	NA	Full	60.278	0.719	-1.019
CARS	SG	PLS	1	PCA	106.300	0.125	-0.633
CARS	SG	RF	NA	PCA	62.799	0.695	-0.319
CARS	SG	SVM	NA	PCA	106.496	0.122	-0.747
CARS	SG	ANN	NA	PCA	109.673	0.068	-0.770
CARS	MSC	PLS	3	Full	87.908	0.401	-0.324
CARS	MSC	RF	NA	Full	23.351	0.958	-0.025
CARS	MSC	SVM	NA	Full	113.802	-0.003	-0.688
CARS	MSC	ANN	NA	Full	114.136	-0.009	-0.873
CARS	MSC	PLS	1	PCA	105.543	0.137	-1.193
CARS	MSC	RF	NA	PCA	45.983	0.836	-0.530
CARS	MSC	SVM	NA	PCA	100.508	0.218	-0.658
CARS	MSC	ANN	NA	PCA	105.301	0.141	-0.802

CARS	SNV+SG	PLS	3	Full	86.871	0.415	-0.220
CARS	SNV+SG	RF	NA	Full	35.821	0.901	0.112
CARS	SNV+SG	SVM	NA	Full	112.429	0.021	-0.753
CARS	SNV+SG	ANN	NA	Full	71.793	0.601	-0.698
CARS	SNV+SG	PLS	1	PCA	112.332	0.023	-0.669
CARS	SNV+SG	RF	NA	PCA	131.653	-0.343	-1.178
CARS	SNV+SG	SVM	NA	PCA	111.740	0.033	-0.908
CARS	SNV+SG	ANN	NA	PCA	114.226	-0.011	-0.648
RandomFrog	SNV	PLS	4	Full	87.252	0.410	-0.414
RandomFrog	SNV	RF	NA	Full	20.482	0.968	-0.174
RandomFrog	SNV	SVM	NA	Full	113.899	-0.005	-0.687
RandomFrog	SNV	ANN	NA	Full	70.031	0.620	-0.585
RandomFrog	SNV	PLS	1	PCA	105.574	0.137	-1.263
RandomFrog	SNV	RF	NA	PCA	42.657	0.859	-0.361
RandomFrog	SNV	SVM	NA	PCA	100.208	0.222	-0.714
RandomFrog	SNV	ANN	NA	PCA	62.758	0.695	-0.469
RandomFrog	SG	PLS	3	Full	84.960	0.441	-0.351
RandomFrog	SG	RF	NA	Full	21.516	0.964	0.153
RandomFrog	SG	SVM	NA	Full	111.642	0.035	-0.733
RandomFrog	SG	ANN	NA	Full	101.287	0.205	-0.754
RandomFrog	SG	PLS	1	PCA	104.636	0.152	-0.579
RandomFrog	SG	RF	NA	PCA	69.025	0.631	-0.233
RandomFrog	SG	SVM	NA	PCA	105.497	0.138	-0.702
RandomFrog	SG	ANN	NA	PCA	108.964	0.080	-0.782
RandomFrog	MSC	PLS	4	Full	82.152	0.477	-0.432
RandomFrog	MSC	RF	NA	Full	23.346	0.958	-0.342
RandomFrog	MSC	SVM	NA	Full	113.898	-0.005	-0.687

RandomFrog	MSC	ANN	NA	Full	80.021	0.504	-0.599
RandomFrog	MSC	PLS	1	PCA	105.648	0.135	-1.264
RandomFrog	MSC	RF	NA	PCA	43.454	0.854	-0.363
RandomFrog	MSC	SVM	NA	PCA	100.263	0.221	-0.714
RandomFrog	MSC	ANN	NA	PCA	105.398	0.140	-0.940
RandomFrog	SNV+SG	PLS	3	Full	88.731	0.390	-0.346
RandomFrog	SNV+SG	RF	NA	Full	22.830	0.960	-0.075
RandomFrog	SNV+SG	SVM	NA	Full	111.887	0.030	-0.751
RandomFrog	SNV+SG	ANN	NA	Full	85.032	0.440	-0.623
RandomFrog	SNV+SG	PLS	1	PCA	104.161	0.160	-0.586
RandomFrog	SNV+SG	RF	NA	PCA	79.491	0.511	-0.287
RandomFrog	SNV+SG	SVM	NA	PCA	107.964	0.097	-0.807
RandomFrog	SNV+SG	ANN	NA	PCA	104.145	0.160	-0.577