

Permutation Results

Probability of Model Insignificance vs. Permuted Samples
For model with 4 component(s)

Y-column: 1

	Wilcoxon	Sign Test	Rand t-test
Self-Prediction:	0.003	0.043	0.005
Cross-Validated:	0.001	0.016	0.005

Y-column: 2

	Wilcoxon	Sign Test	Rand t-test
Self-Prediction:	0.003	0.043	0.005
Cross-Validated:	0.001	0.016	0.005

Values less than 0.05 indicate the model is significant at the 95% confidence level.

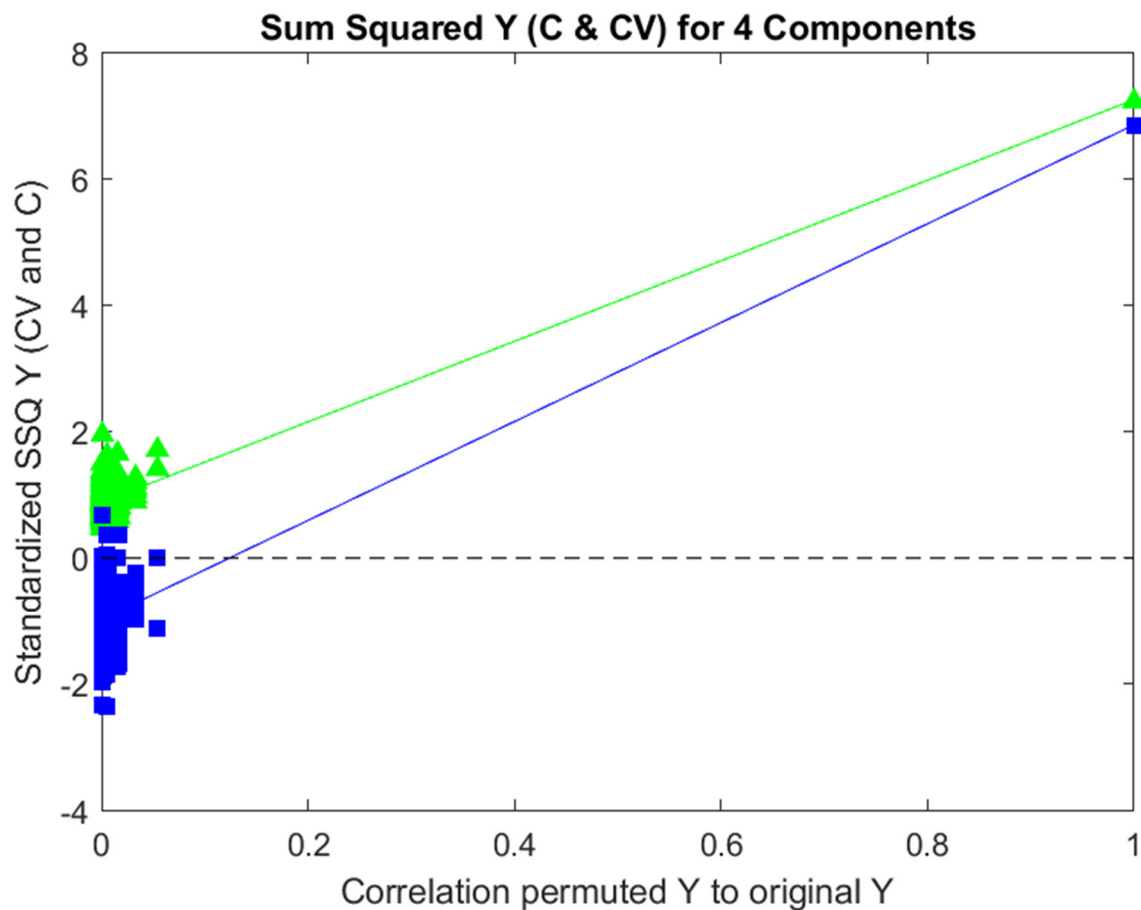


Figure S3a. Permutation test (n=200) of PLS-DA model Y-column 1 and 2.

Permutation Results

Probability of Model Insignificance vs. Permuted Samples
For model with 5 component(s)

Y-column: 1

	Wilcoxon	Sign Test	Rand t-test
Self-Prediction:	0.000	0.000	0.005
Cross-Validated:	0.000	0.000	0.005

Values less than 0.05 indicate the model is significant at the 95% confidence level.

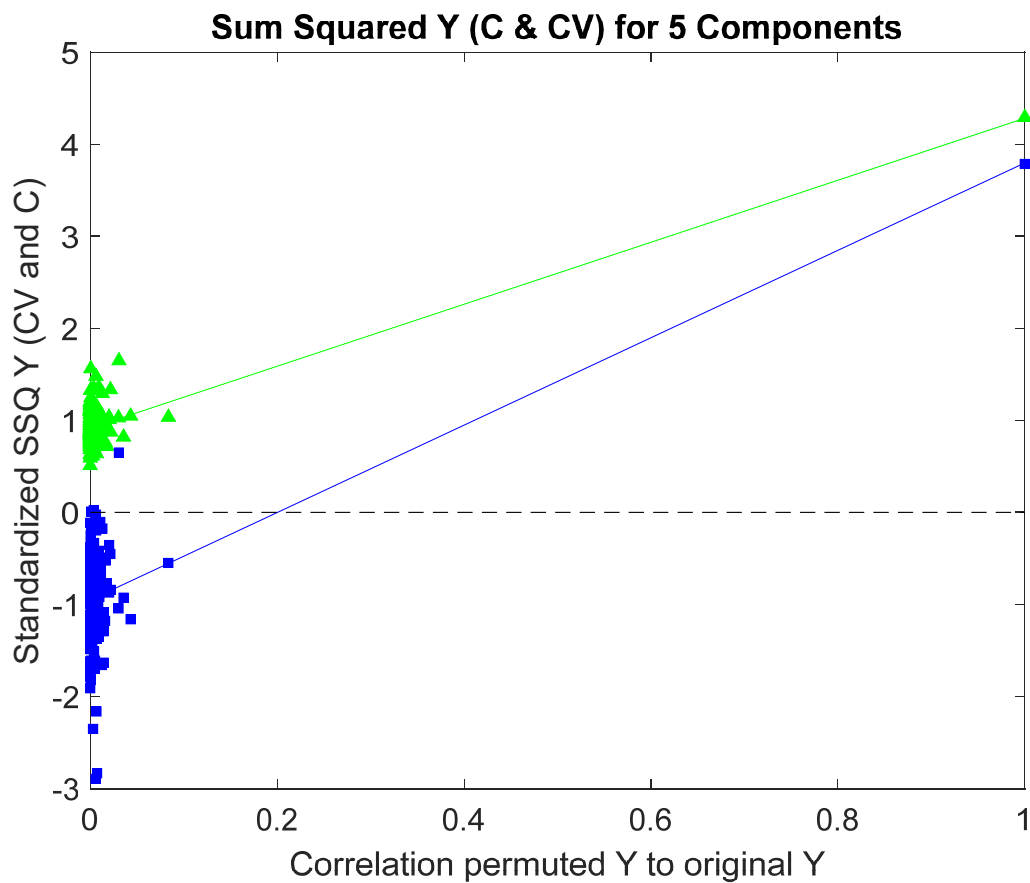


Figure S3b. Permutation test (n=200) of (a) PLS-R model where the R^2 prediction = 0.78

Permutation Results

Probability of Model Insignificance vs. Permuted Samples
For model with 5 component(s)

Y-column: 1

	Wilcoxon	Sign Test	Rand t-test
Self-Prediction:	0.000	0.000	0.005
Cross-Validated:	0.000	0.000	0.005

Values less than 0.05 indicate the model is significant at the 95% confidence level.

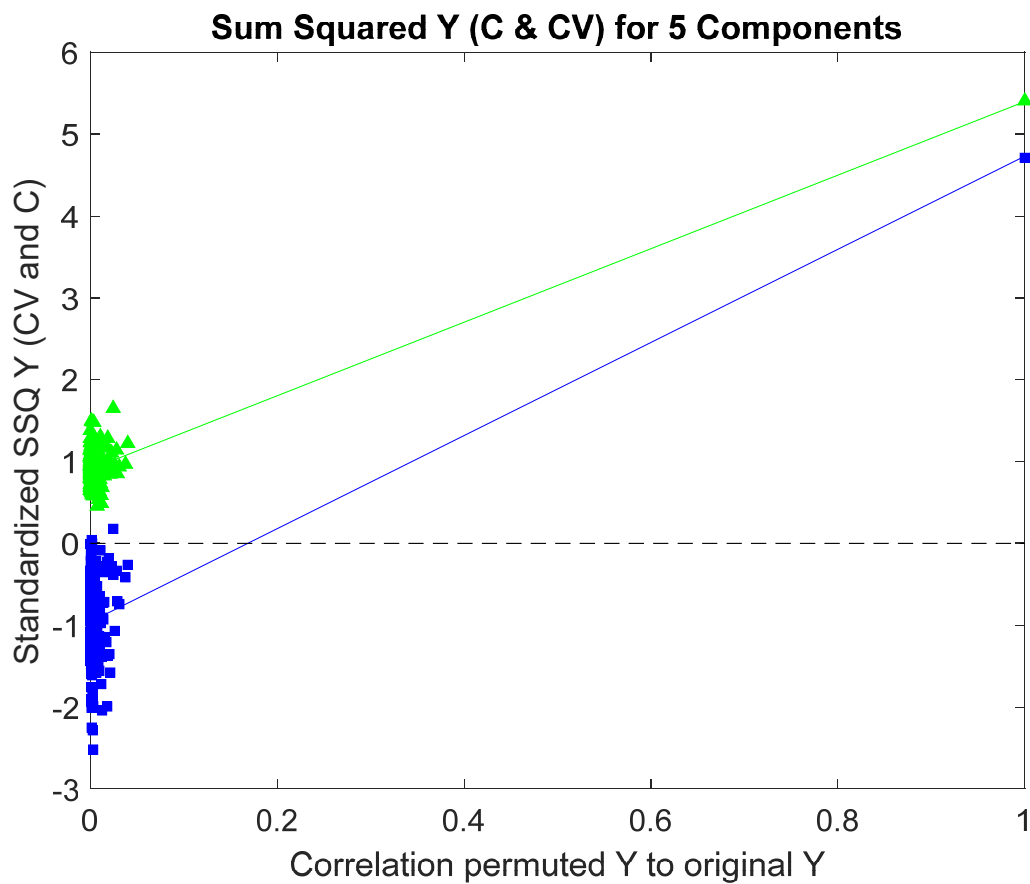


Figure S3c. Permutation test (n=200) of (b) PLS-R model where the R^2 prediction = 0.75

Permutation Results

Probability of Model Insignificance vs. Permuted Samples
For model with 4 component(s)

Y-column: 1

	Wilcoxon	Sign Test	Rand t-test
Self-Prediction:	0.000	0.000	0.005
Cross-Validated:	0.000	0.000	0.005

Values less than 0.05 indicate the model is significant at the 95% confidence level.

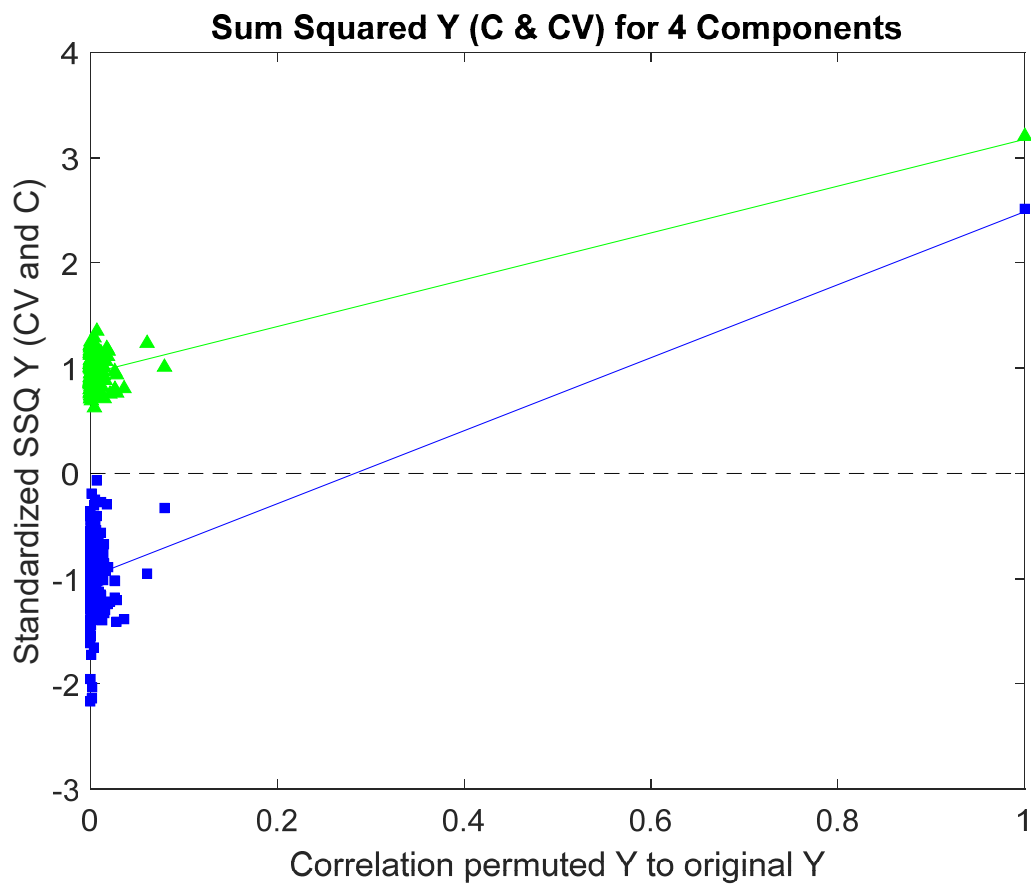


Figure S3d. Permutation test (n=200) of (c) PLS-R model where the R^2 prediction = 0.73

Permutation Results

Probability of Model Insignificance vs. Permuted Samples

Y-column: 1

	Wilcoxon	Sign Test	Rand t-test
Self-Prediction:	0.111	0.117	0.009
Cross-Validated:	0.000	0.000	0.005

Values less than 0.05 indicate the model is significant at the 95% confidence level.

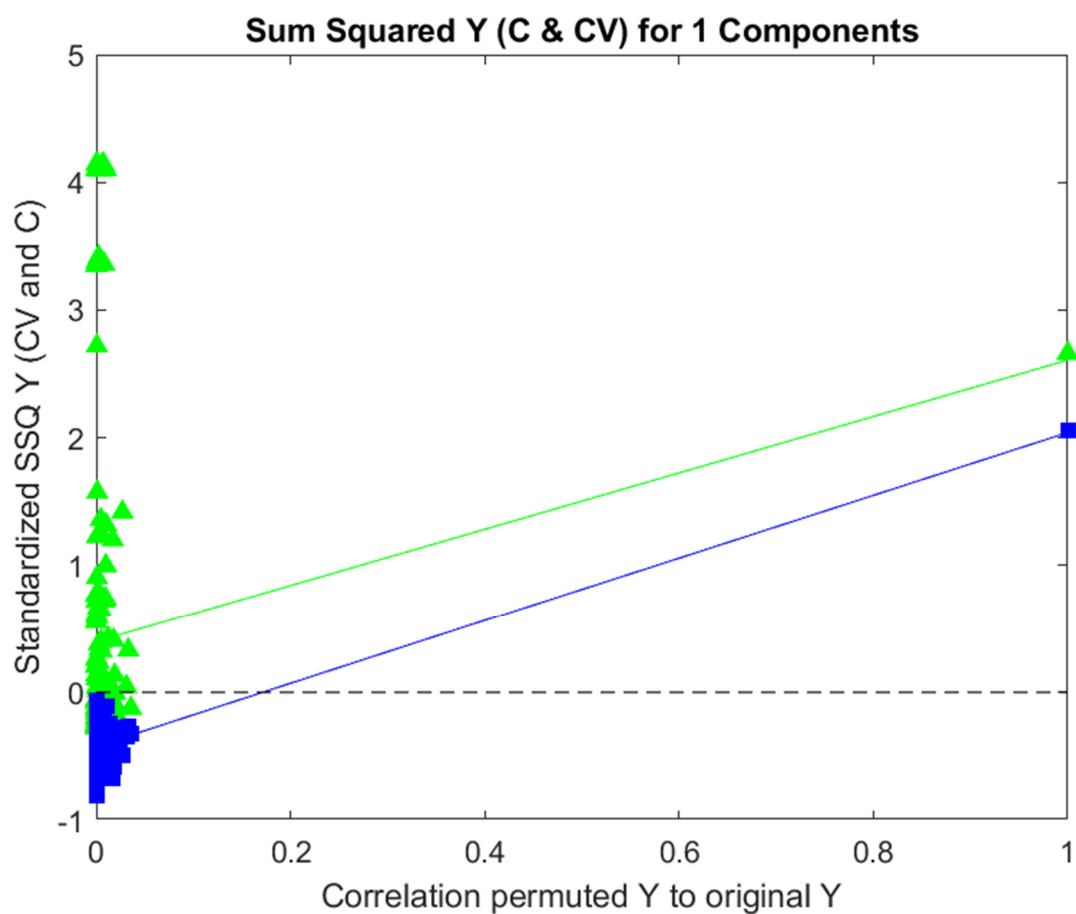


Figure S3e. Permutation test (n=200) of (a) SVM-R model where the R^2 prediction = 0.77

Permutation Results

Probability of Model Insignificance vs. Permuted Samples

Y-column: 1

	Wilcoxon	Sign Test	Rand t-test
Self-Prediction:	0.035	0.036	0.005
Cross-Validated:	0.000	0.000	0.005

Values less than 0.05 indicate the model is significant at the 95% confidence level.

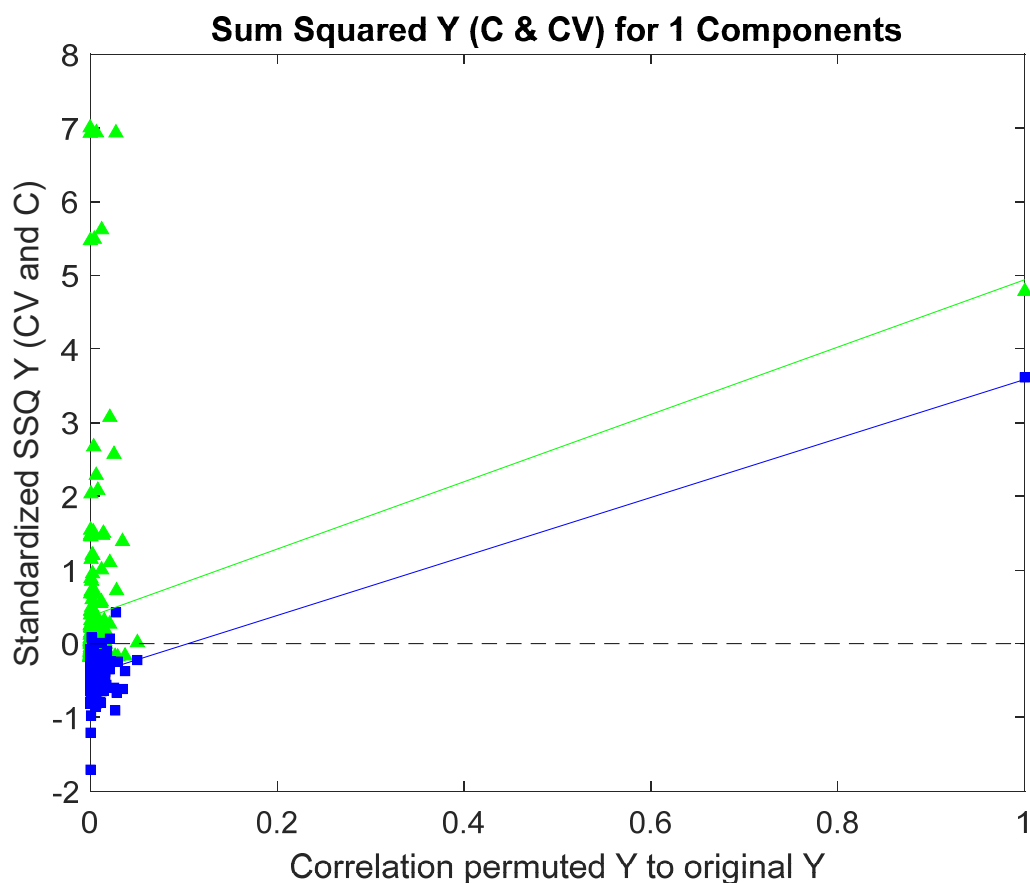


Figure S3f. Permutation test (n=200) of (c) SVM-R model where the R^2 prediction = 0.76

Permutation Results

Probability of Model Insignificance vs. Permuted Samples

Y-column: 1

	Wilcoxon	Sign Test	Rand t-test
Self-Prediction:	0.100	0.100	0.005
Cross-Validated:	0.000	0.000	0.005

Values less than 0.05 indicate the model is significant at the 95% confidence level.

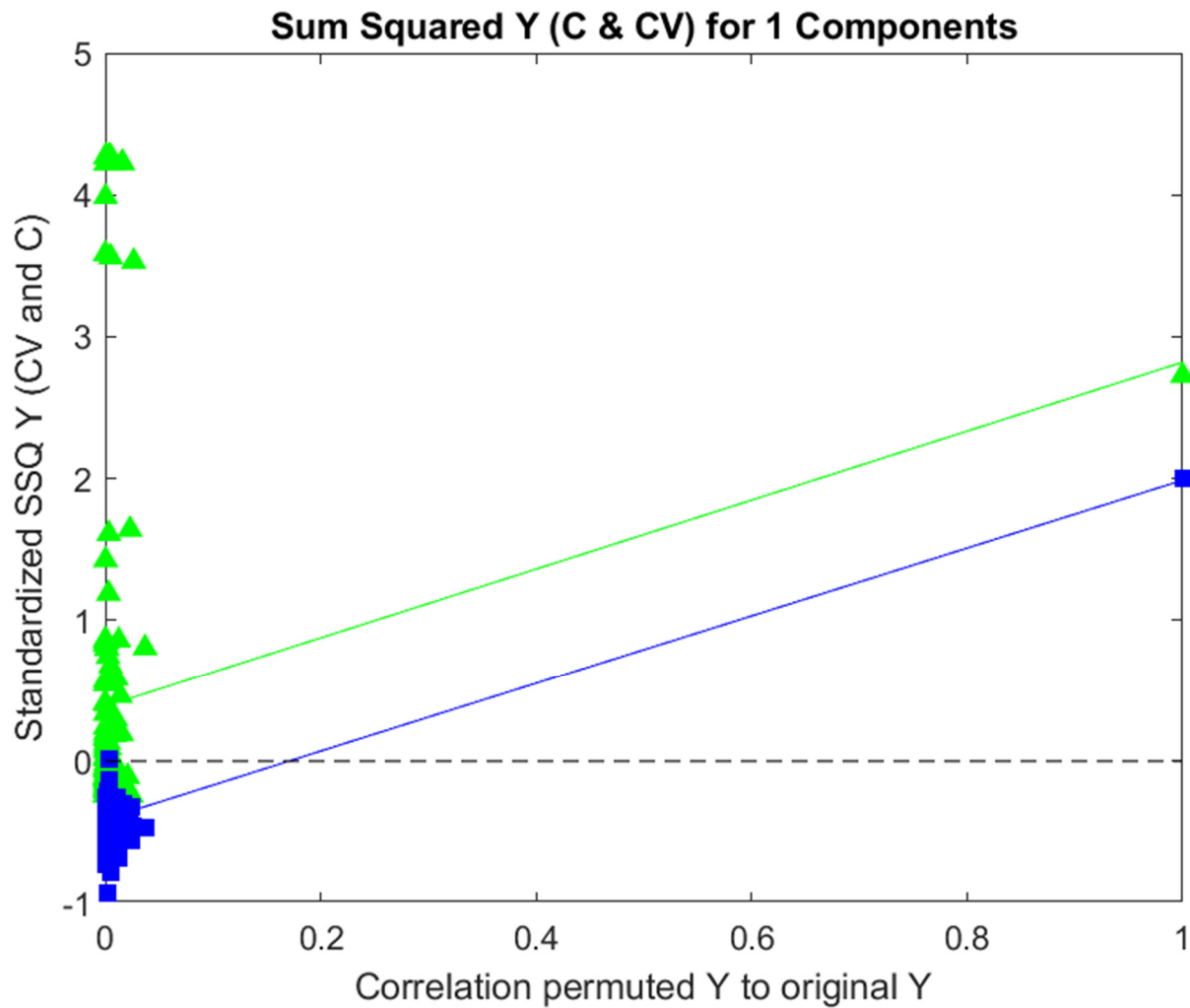


Figure S3g. Permutation test (n=200) of (b) SVM-R model where the R^2 prediction = 0.74

Permutation Results

Probability of Model Insignificance vs. Permuted Samples

Y-column: 1

	Wilcoxon	Sign Test	Rand t-test
Self-Prediction:	0.000	0.000	0.005
Cross-Validated:	0.000	0.000	0.005

Values less than 0.05 indicate the model is significant at the 95% confidence level.

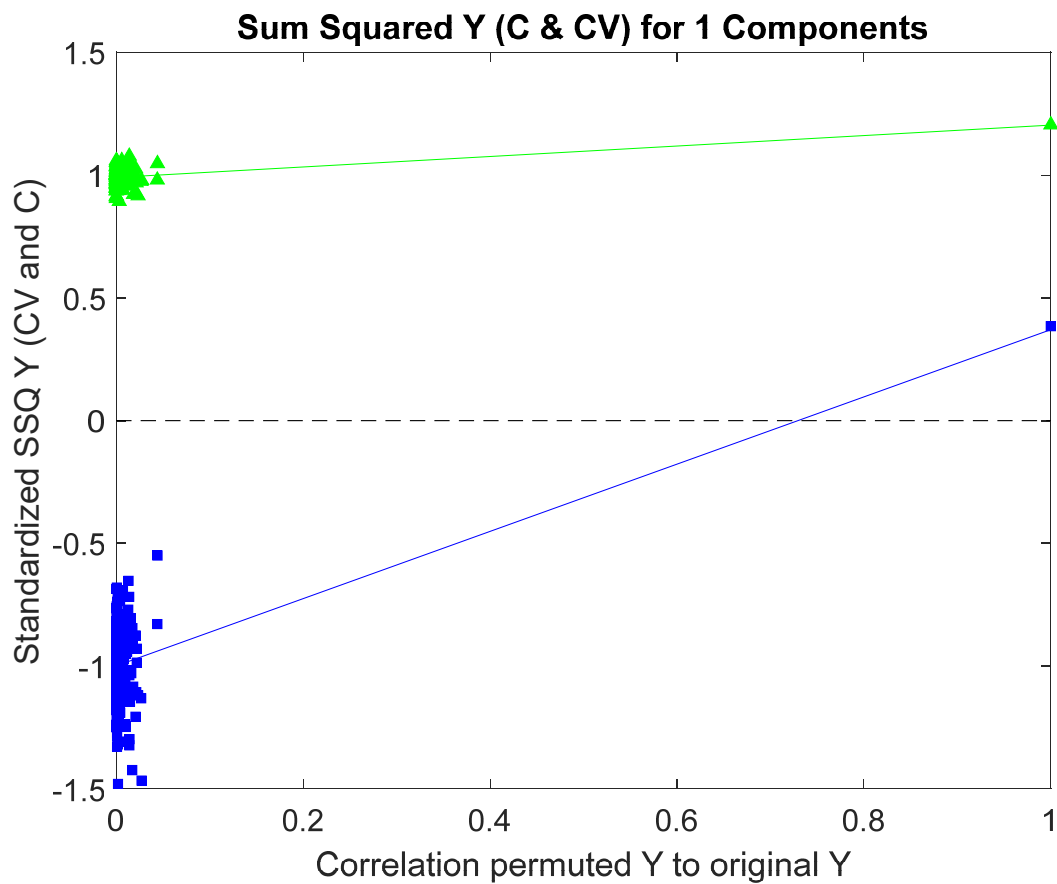


Figure S3h. Permutation test (n=200) of (a) XGB-R model where the R^2 prediction = 0.74

Permutation Results

Probability of Model Insignificance vs. Permuted Samples

Y-column: 1

	Wilcoxon	Sign Test	Rand t-test
Self-Prediction:	0.386	0.389	0.626
Cross-Validated:	0.000	0.000	0.005

Values less than 0.05 indicate the model is significant at the 95% confidence level.

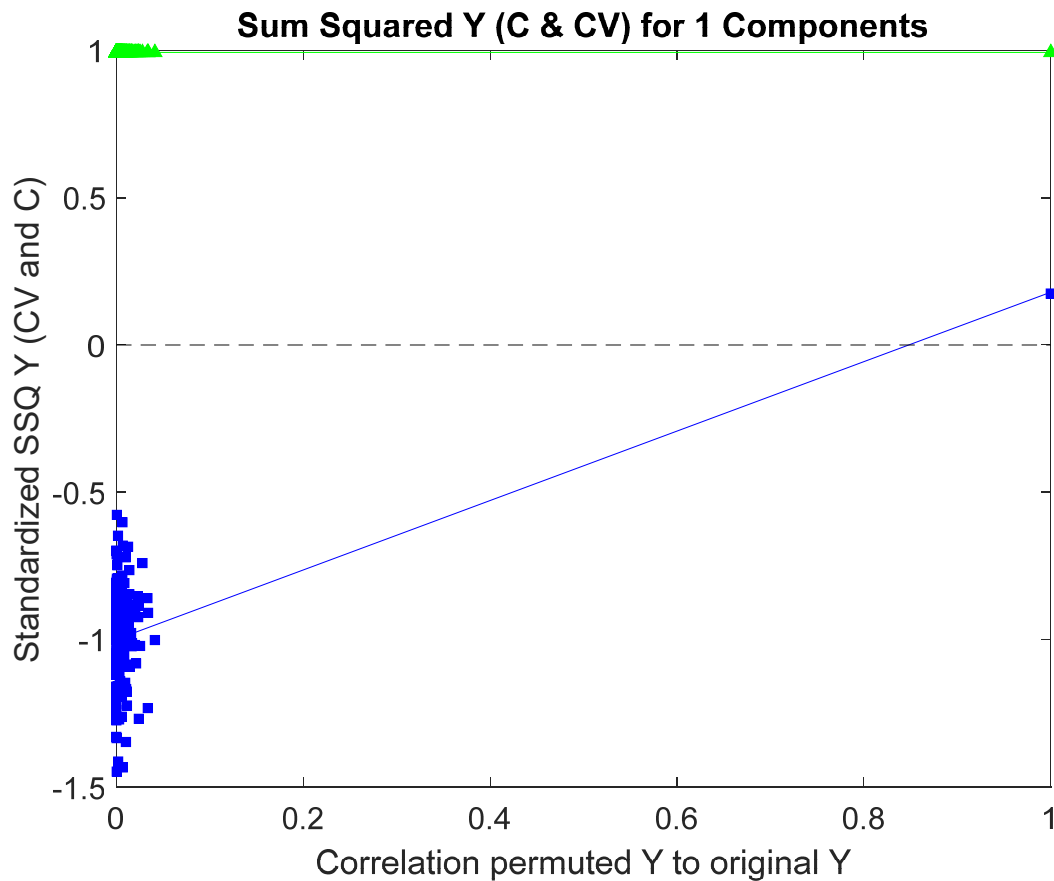


Figure S3i. Permutation test (n=200) of (a) XGB-R model where the R^2 prediction = 0.59

Permutation Results

Probability of Model Insignificance vs. Permuted Samples

Y-column: 1

	Wilcoxon	Sign Test	Rand t-test
Self-Prediction:	0.001	0.005	0.010
Cross-Validated:	0.000	0.000	0.005

Values less than 0.05 indicate the model is significant at the 95% confidence level.

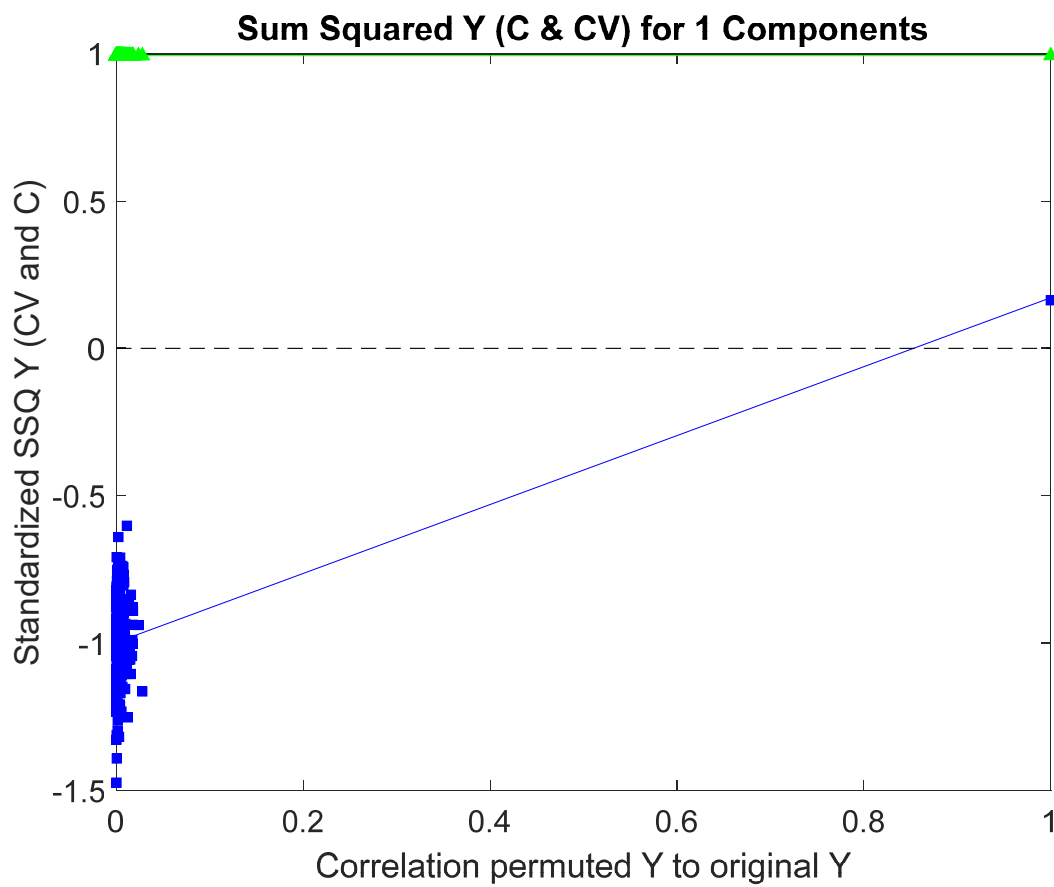


Figure S3j. Permutation test (n=200) of (a) XGB-R model where the R^2 prediction = 0.74