

Supplementary Information

Raman hyperspectroscopy of saliva and machine learning for Sjögren's Syndrome diagnostics

Bhavik Vyas¹, Ana Khatiaashvili², Lisa Galati², Khoa Ngo², Neil Gildener-Leapman², Melinda Larsen³ and Igor K. Lednev^{1,3*}

¹Department of Chemistry, University at Albany, SUNY, Albany, NY 12222

²Division of Otolaryngology Head and Neck Surgery, Albany Medical College, Albany NY 12208

³Department of Biology and The RNA Institute, University at Albany, SUNY, Albany, NY 12222

*Corresponding Author: ilednev@albany.edu

Fig S1. Outlier removal using Hotelling T². The spectra with the T² Hotelling values exceeding reduced statistical threshold (--) considered outliers (Grey area top right)

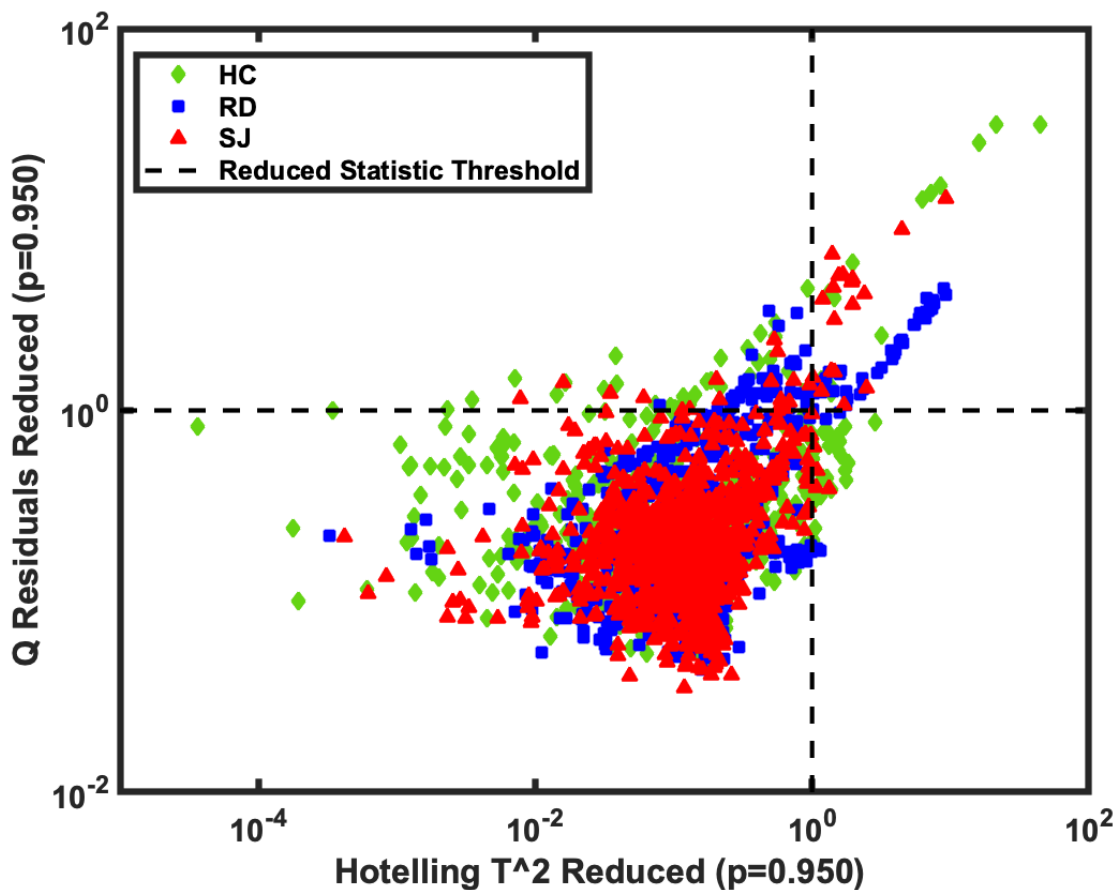


Table S1A. Confusion matrix of the external validation at the spectral level

Predicted Class	Actual Class		
	HC	RD	SJ
HC	74	4	19
RD	5	70	1
SJ	20	7	65

Table S1B. Classification predictions for individual spectra collected for each of the nine samples used for external validation.

True class	Predicted class		
	HC	RD	SjD
HC-1	32	3	1
HC-2	20	1	11
HC-3	22	1	8
RD-1	4	21	2
RD-2	0	19	4
RD-3	0	30	1
SjD-1	6	1	11
SjD-2	0	0	37
SjD-3	13	0	17