

SUPPLEMENTARY MATERIALS

Supp. 1 Data for Figure 2 : Effect of outlier removal and averaging of spectra.

	Without outlier removal, without averaging			With outlier removal, without averaging			With outlier removal, with averaging (5)		
	Sens.	Std Sens.	Spec.	Sens.	Std. Sens.	Spec.	Sens.	Std Sens.	Spec.
BC	98.3	1.23	99.3	99.0	0.5	99.7	100	0	100
BS	96.9	2.44	99.6	98.7	1	99.7	100	0	100
SE	98.9	0.98	99.8	100	0	99.9	100	0	100
EC	85.5	7.2	94.7	87.1	5.3	96	93.8	3.5	98.1
SM	79.1	9	96.3	84.1	8.9	96.8	90.3	6	94.3

Sens. = sensitivity (true-positive), Spec. = specificity (true-negative), Std. Sens = standard deviation of sensitivity over 10 classifications.