

Sample preparation

Raman measurements that were used in the data model come from samples that were acquired from the Academic Medical Center (AMC) and National Institute for Public Health and the Environment (RIVM). The human samples are all used for PCR and their corresponding Ct values are known. The human samples from the AMC were stored at -80 Celsius degrees in Eswab, VVM, UTM or GLY medium. When the human samples were thawed, these were centrifuged at a speed of 10000 RPM for 5 minutes. In this centrifugation step, the saliva cells will go down to form a pellet and the virus particles will stay up in the supernatant. The supernatant is diluted in a ratio of 1:10 with ethanol. 10 ul of the diluted sample is pipetted onto the chip. The analyte is dried for a few minutes. The human samples from the RIVM were stored at -20 Celsius degrees in UTM or GLY medium, and inactivated by heat (1 hour at 60 Celsius degrees). At the Artemis On Health lab the human samples were stored at -80 Celsius degrees. When the human samples were thawed, these were centrifuged at a speed of 10000 RPM for 5 minutes. The supernatant is diluted in a ratio of 1:10 with ethanol. 10 ul of the diluted sample is pipetted onto the chip. The analyte is dried for a few minutes. After the drying step, Raman measurements are executed with the settings of an acquisition time of 10 seconds and a laser power of 20 mW.

Data

The collected data is shown in table 1. Five sets of each a number of patient samples have been analysed. Each patient sample was measured 3 times on the same chip. In set 2, originally there are more samples but of those the medium is unknown, so they have been left out of the overview and data analysis.

Media	Set 1	Set 2	Set 3	Set 4	Set 5
	RIVM 06/08-04	AMC 23-04 *	AMC 28-04	AMC 04-05	AMC 05-07
ESWAB		288 (96)	261 (87)	144 (48)	96 (32)
VVM			42 (14)		48 (16)
GLY	21 (7)		33 (11)		12 (4)
UTM	33 (11)		30 (10)		36 (12)

Table 1. Number of measurements per medium in each set with between brackets the number of patients used to generate the samples. * Here all samples with unknown media are left out.

Total measurements	
Samples tested as covid positive by PCR	390
Samples tested as covid negative by PCR	654

Preprocessing

As preprocessing we remove all data below 500 nanometers and above 2200 nanometers as at these frequencies we do not see any information

Performance

To estimate the performance of the test a 10-fold cross validation with random shuffle is used. Meaning the data is first randomly shuffled, then the data is split in 10 equally sized groups. Then 10 times 90% of the data used to train and the rest is estimated and evaluated. For each test set we create a Receiver operating characteristic (ROC) curve, this curve shows how changing the cutoff point influences the Specificity and Sensitivity. The Area Under the Curve (AUC) from 0 to 1 of this plot can be used as a general statistic to compare classifier performance.

FOLD NR	1	2	3	4	5	6	7	8	9	10	Total
False Positive (FP)	5	5	2	4	5	4	7	5	6	10	53
True Positive (TP)	32	41	38	26	30	37	29	23	25	35	316
False Negative (FN)	3	7	8	9	10	7	8	6	9	8	75
True Negative (TN)	65	52	57	66	59	56	60	70	64	51	600
Accuracy: (TP + TN) / (TP + FP + TN + FN)	0.924	0.886	0.905	0.876	0.856	0.894	0.856	0.894	0.856	0.827	0.877
Sensitivity: TP / (TP + FN)	0.914	0.854	0.826	0.743	0.750	0.841	0.784	0.793	0.735	0.814	0.808
Specificity: TN / (TN + FP)	0.929	0.912	0.966	0.943	0.922	0.933	0.896	0.933	0.914	0.836	0.919



