

**INTERPRETING RAMAN  
SPECTROSCOPY TOWARDS  
DIAGNOSTIC PURPOSES : AN  
EXPLAINABLE DEEP-LEARNING  
BASED APPROACH**

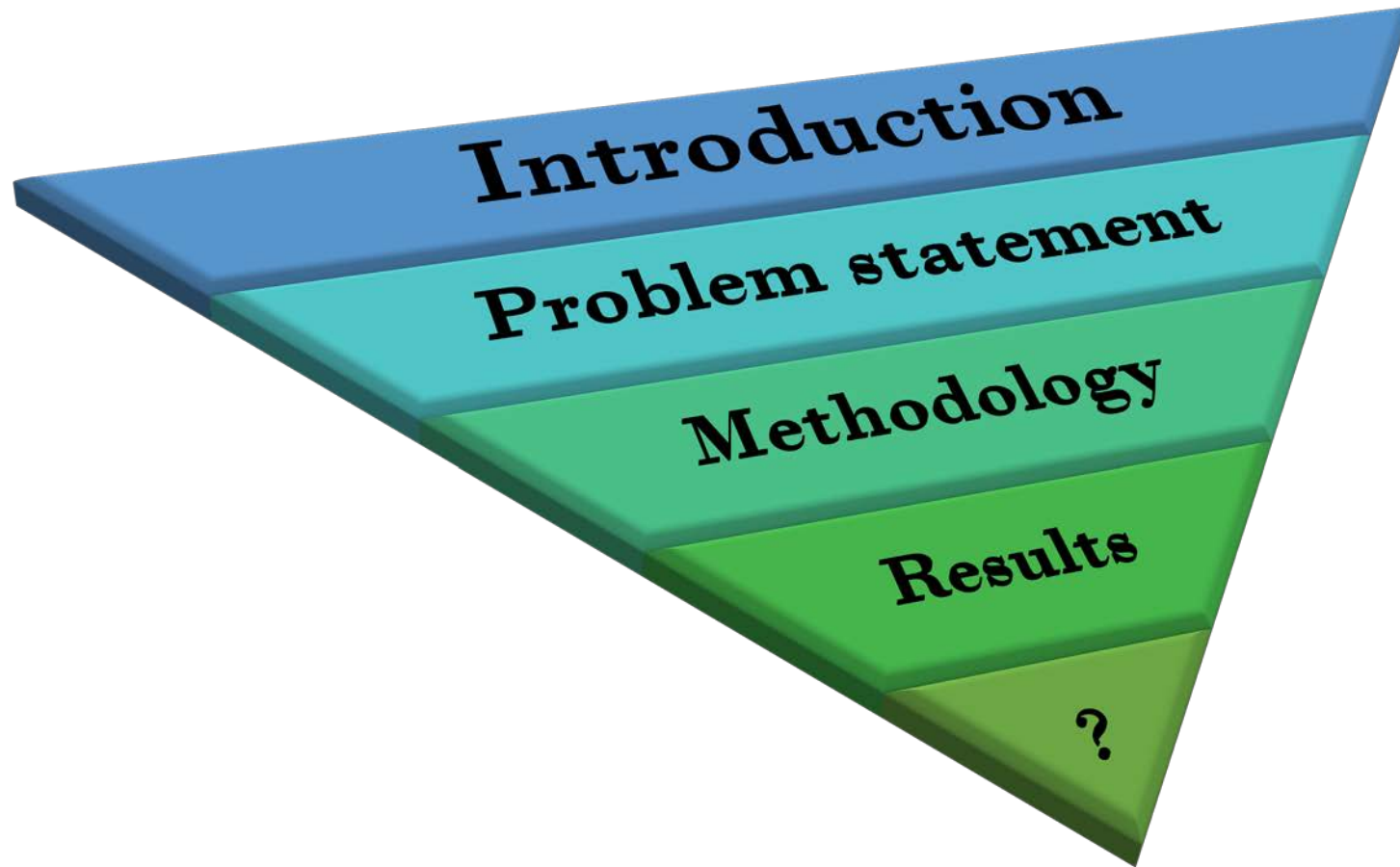
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SINGLAN Nina

Co-Supervisor : Dott. Dario Bertazioli

867646 - 21604881

# OVERVIEW



# INTRODUCTION

# GLOBAL CONTEXT



Need for **non-invasive** and rapid diagnosis system



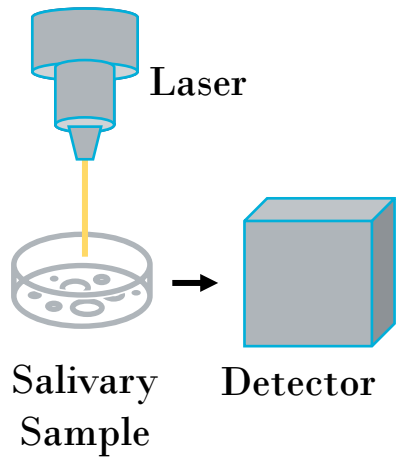
Method called **Raman Spectroscopy** can analyse saliva samples



**Deep Learning** techniques can help to decodes these spectra

# **PROBLEM STATEMENT**

# DATA



## SARS-Cov-2

30 Cov+

+

34 Cov-

+

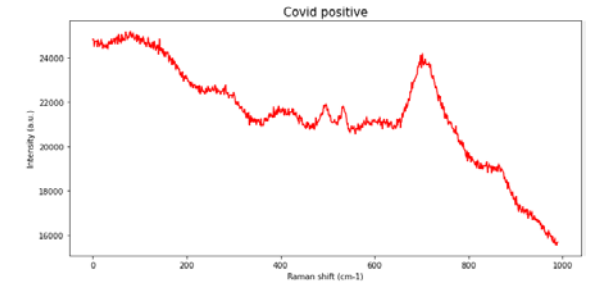
34 CTRLs

=

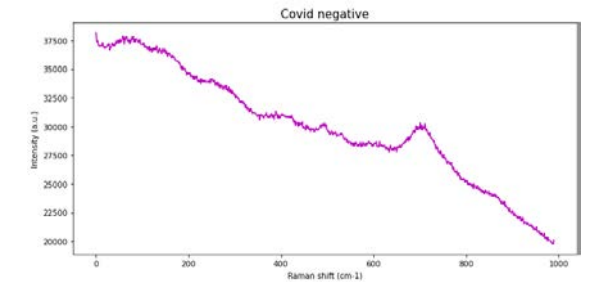
101 patients involved

~ 25 spectra for each patient

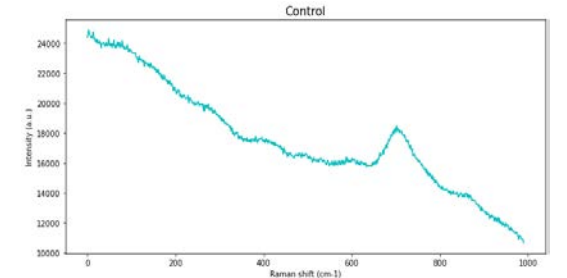
~ 2500 total spectra



Covid Positive

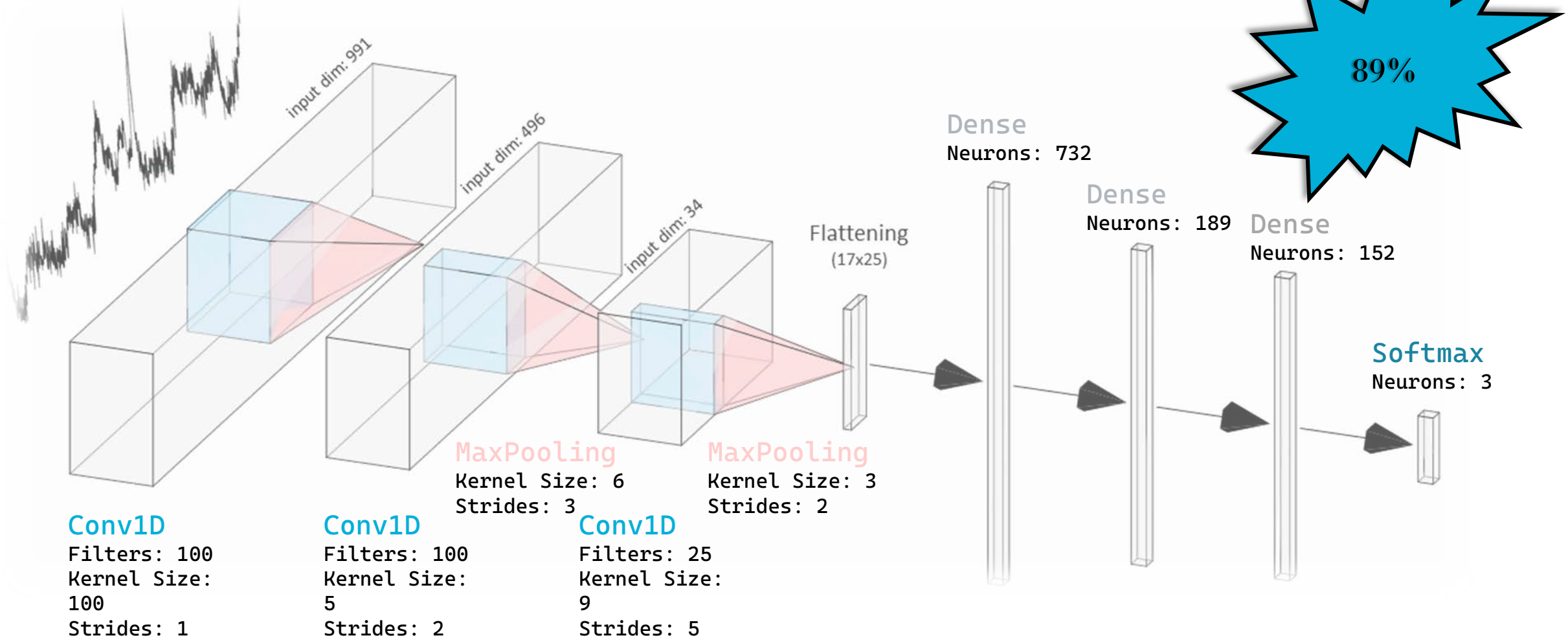


Covid Negative

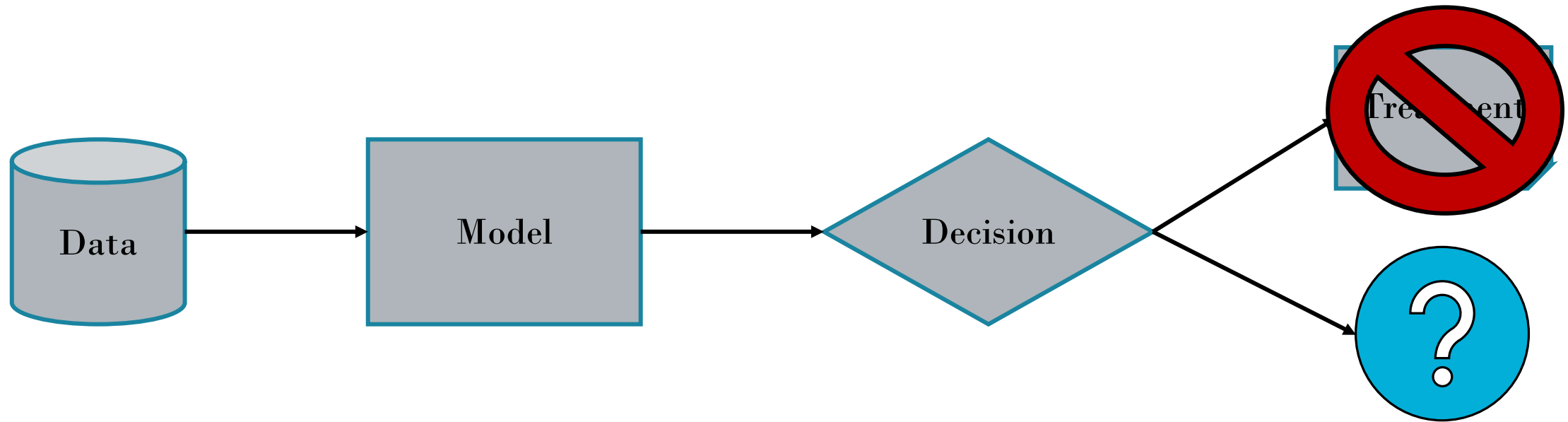


Control

# MODEL



# PROBLEM

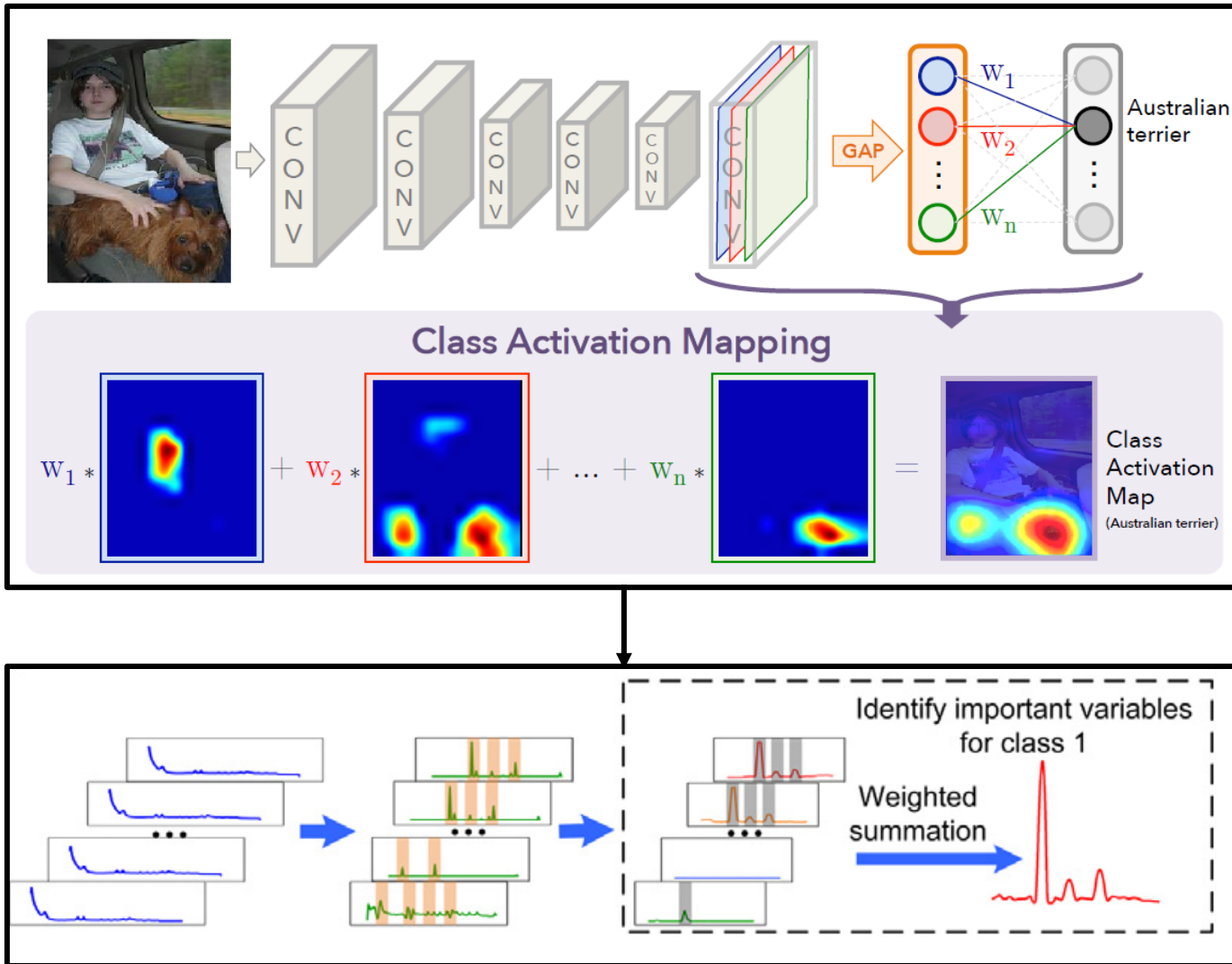


**HOW CAN WE UNDERSTAND THE MODEL AND THEREFORE TRUST IT?**



# **METHODOLOGY**

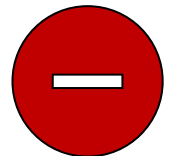
# CLASS ACTIVATION MAPPING



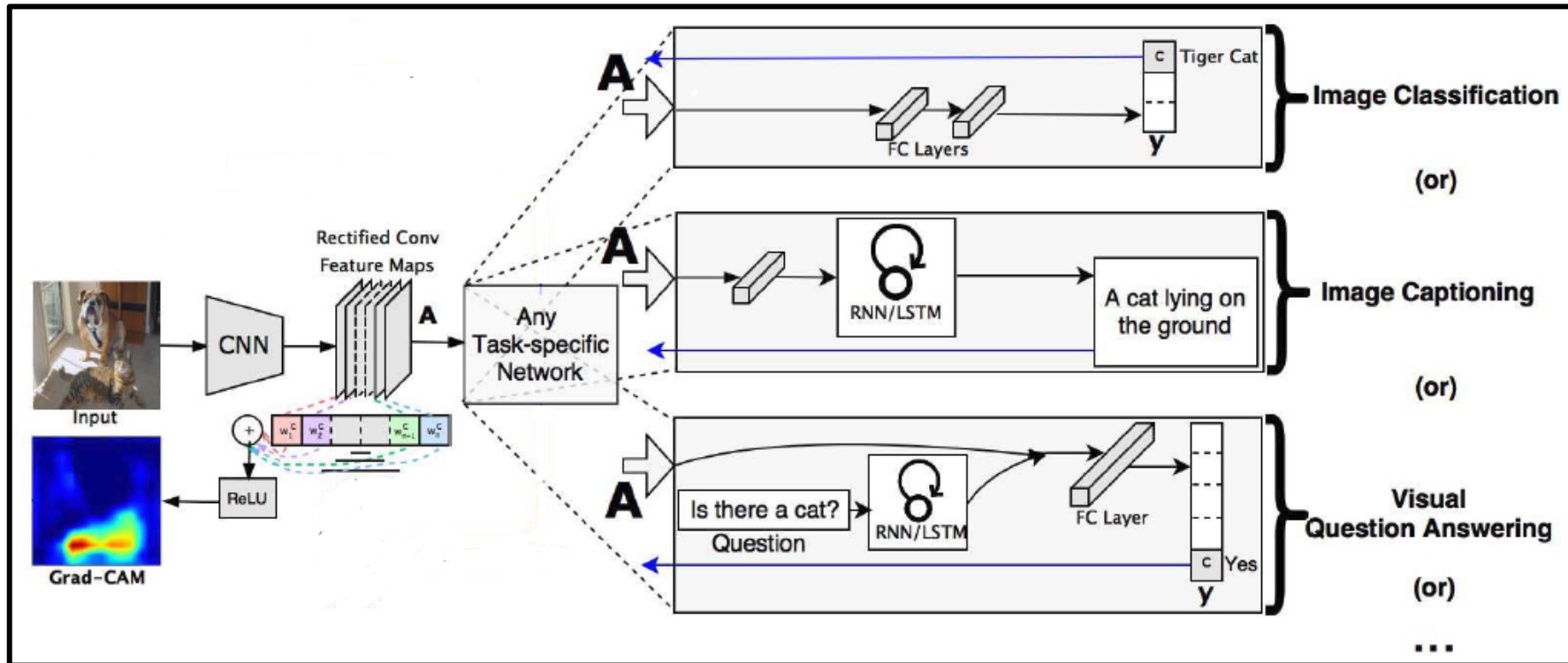
- Already applied to spectra
- Visual explanation



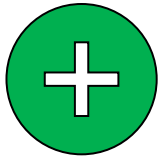
**Need to modify  
and retrain the  
model**



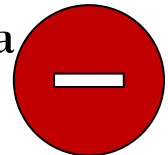
# GRADIENT CAM



**USABLE  
WITH  
EVERY  
CNN**

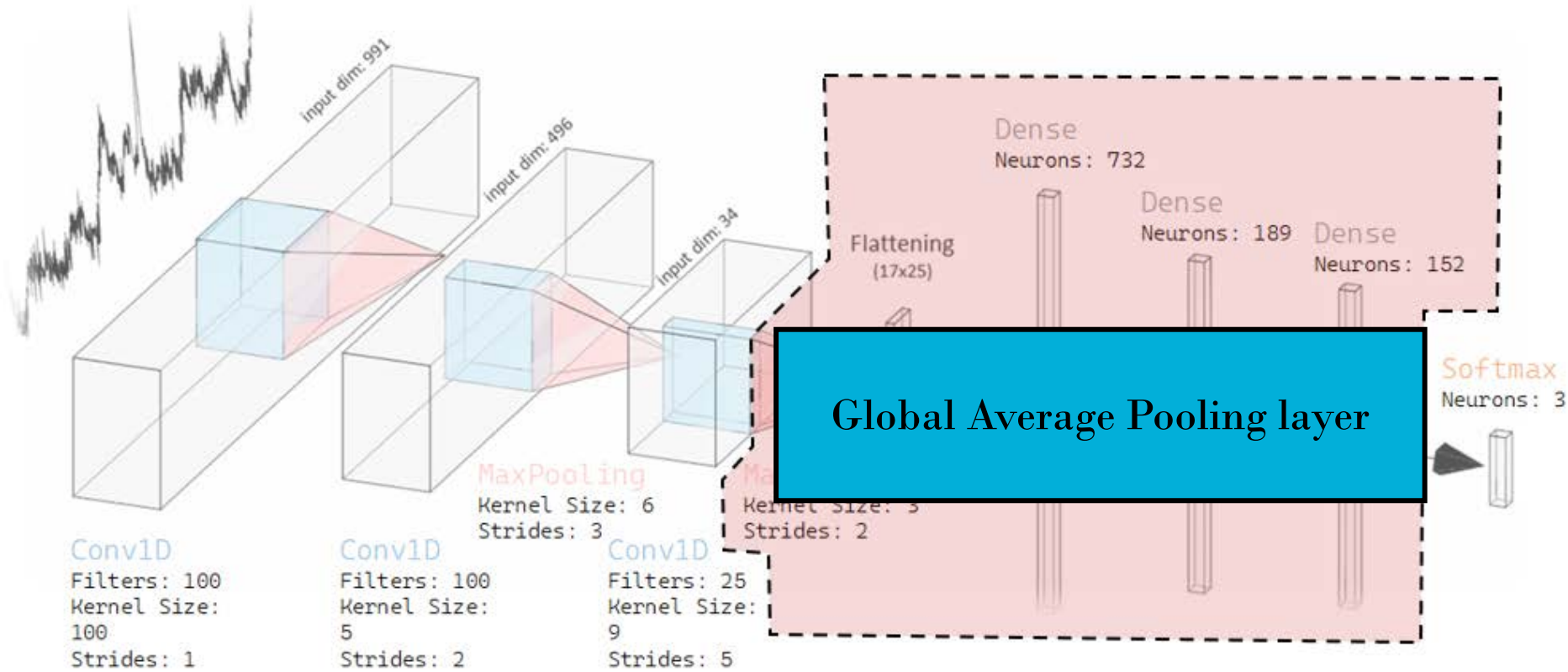


Never applied to  
spectral data



# **RESULTS**

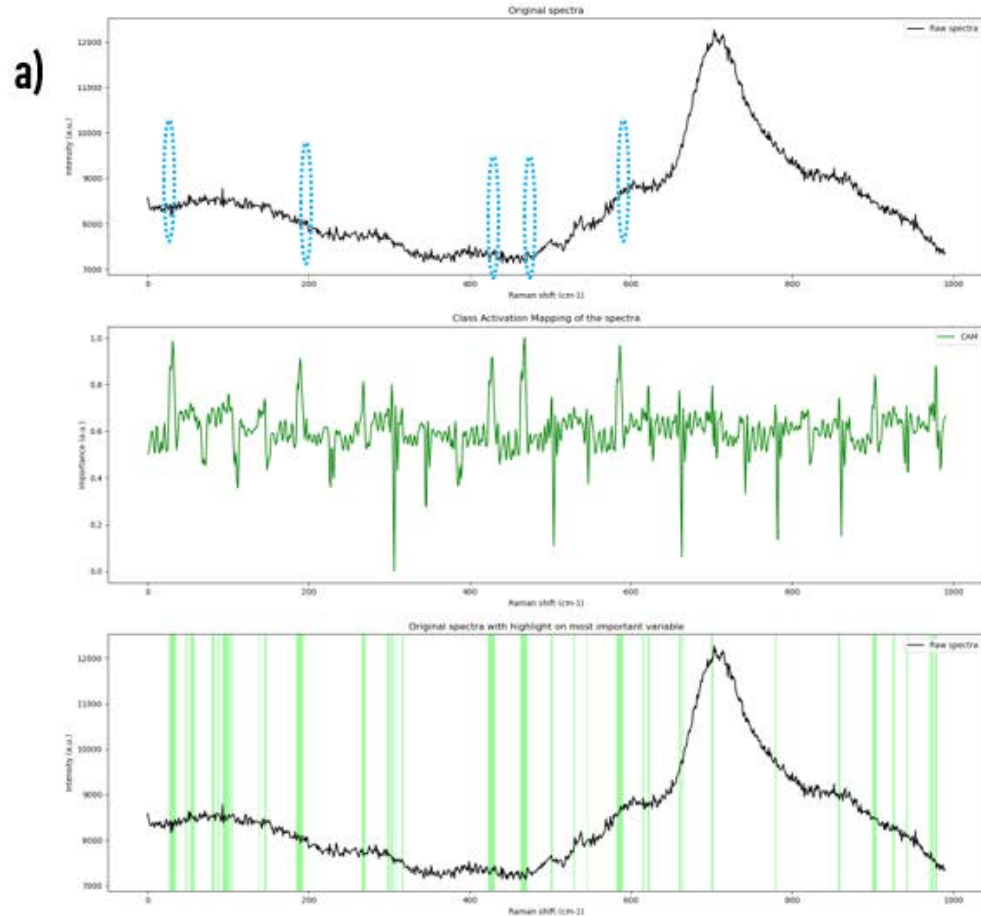
# CAM : CUT MODEL



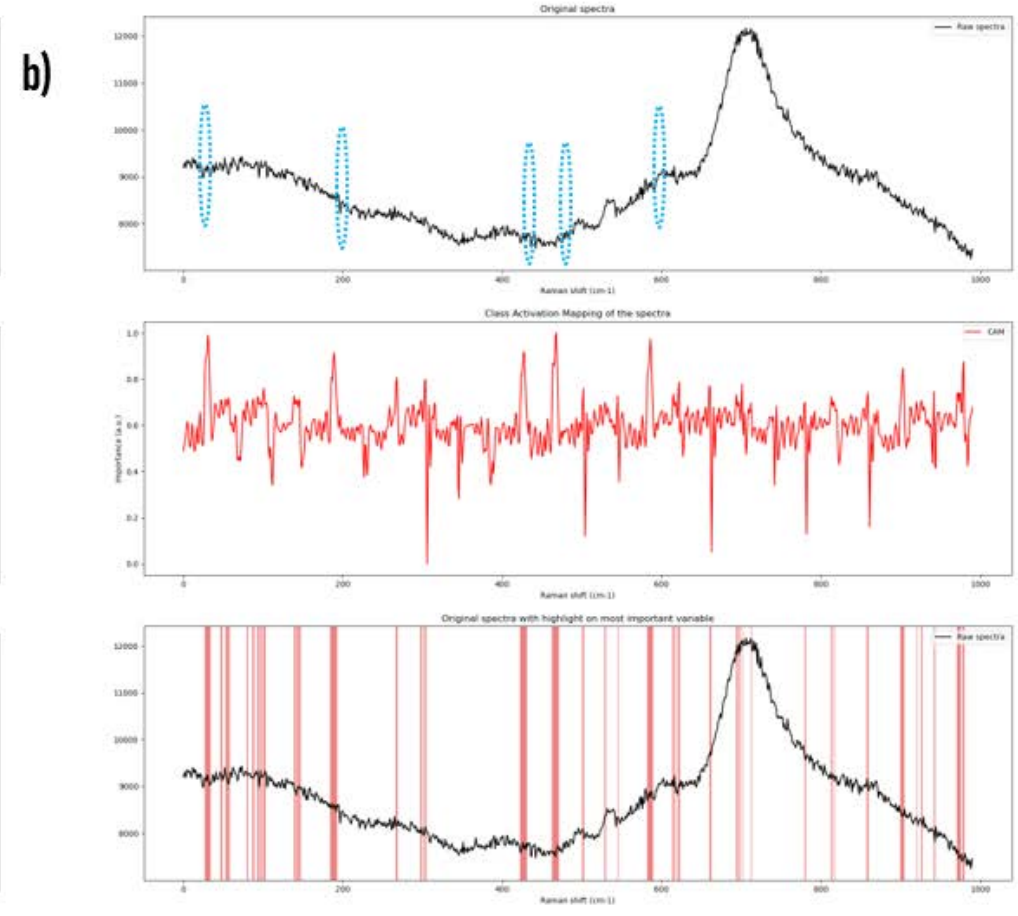
Re-training very  
time consuming !

81.7%

# RESULTS AT SPECTRA LEVEL

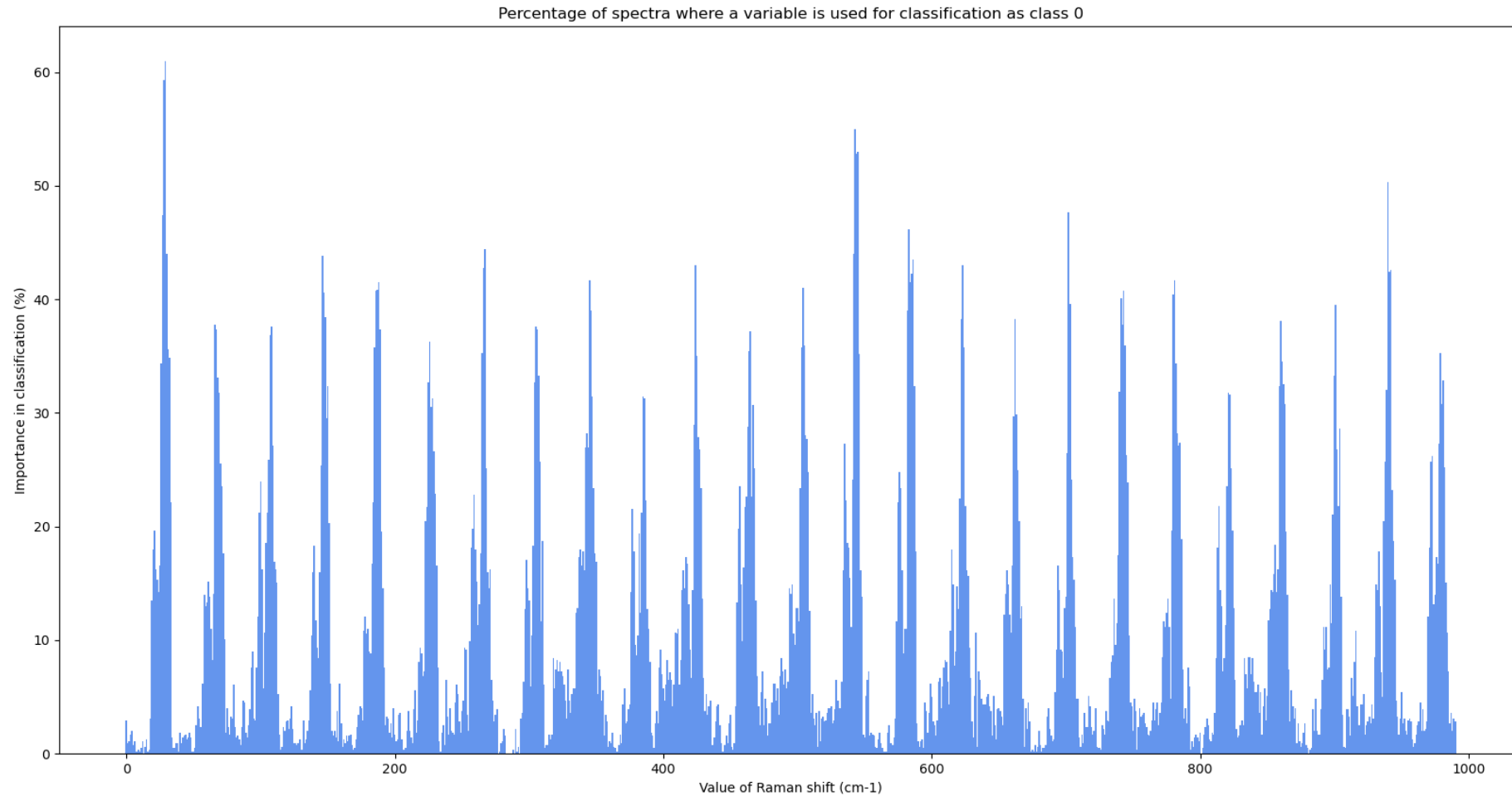


Covid Positive classified as Cov+



Control classified as Cov+

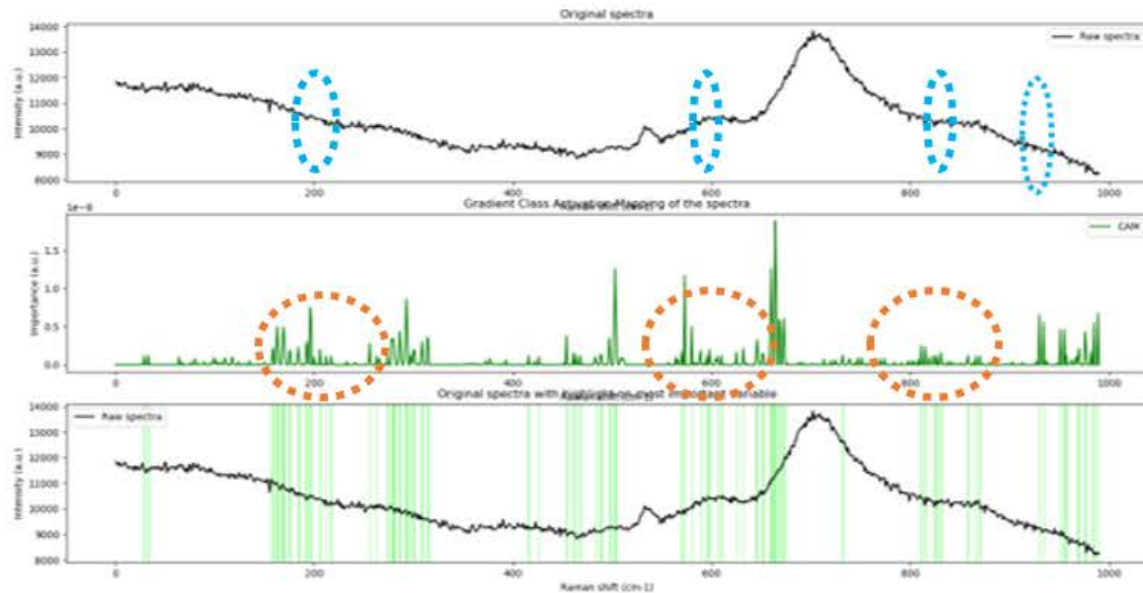
# GENERALIZATION



Number of spectra (%) in which a variable is important for Cov+ classification

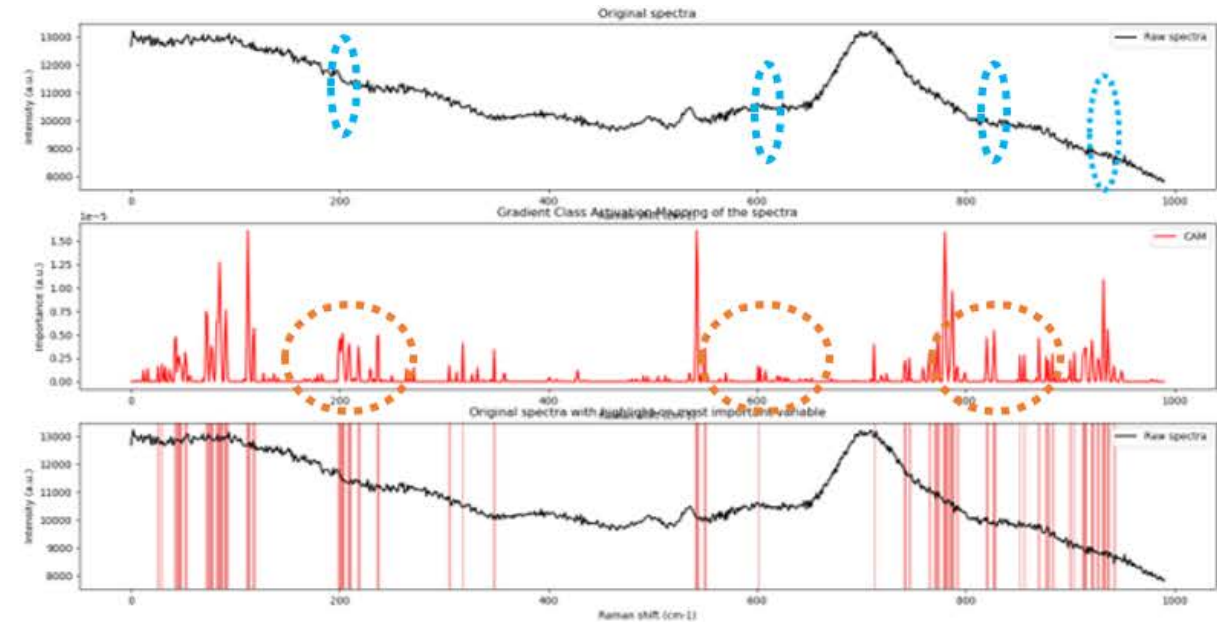
# GRADIENT CAM : RESULTS

a)



Covid Positive classified as Cov+

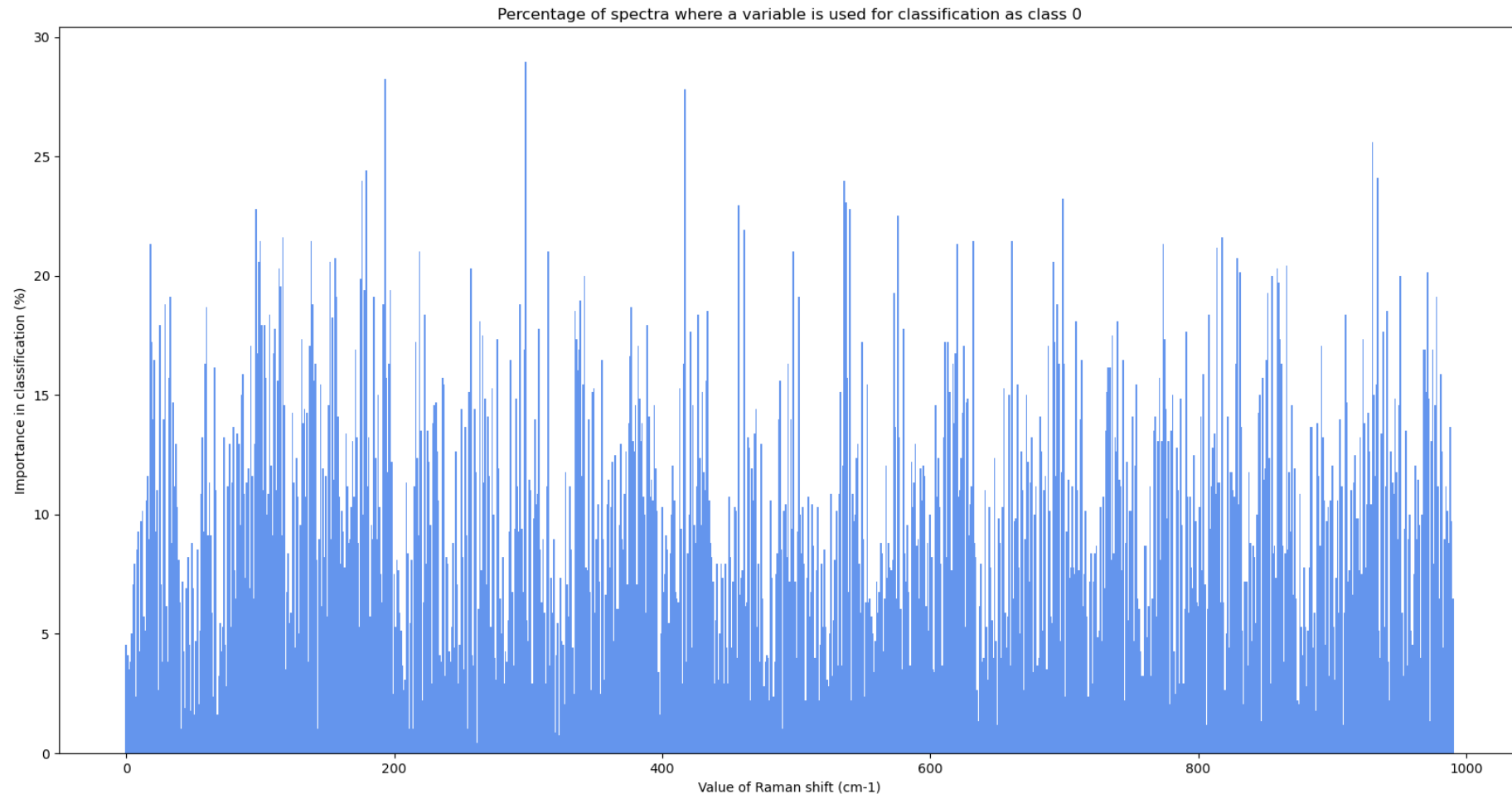
b)



Control classified as Cov+



# GENERALIZATION

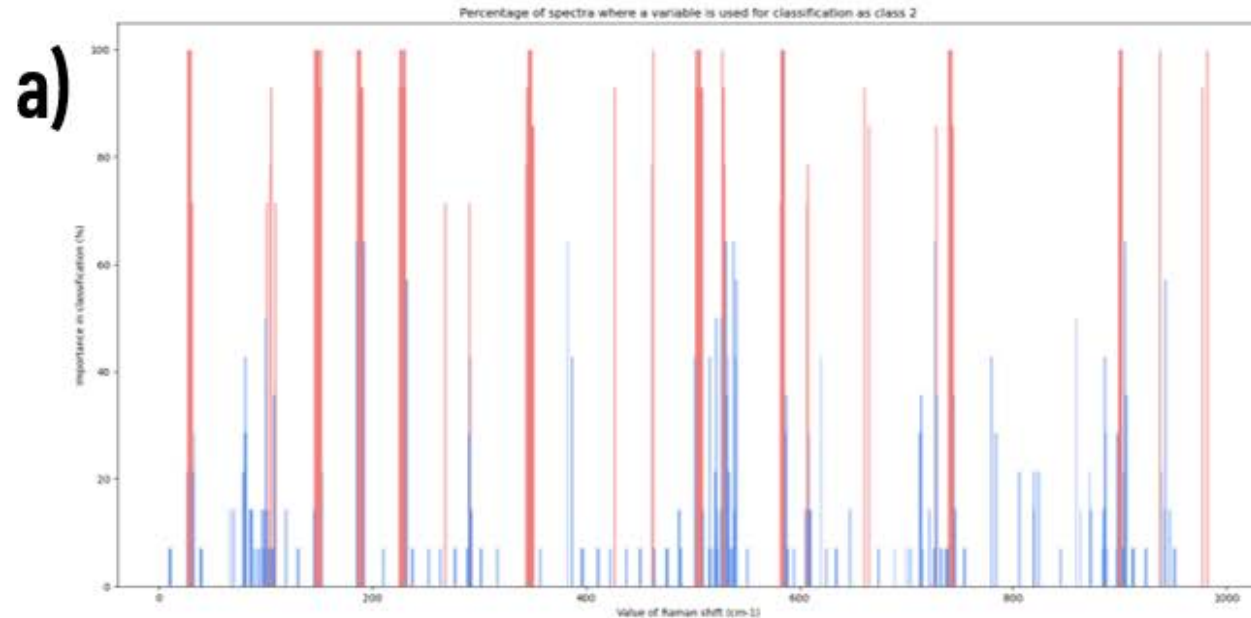


Number of spectra (%) in which a variable is important for Cov+ classification

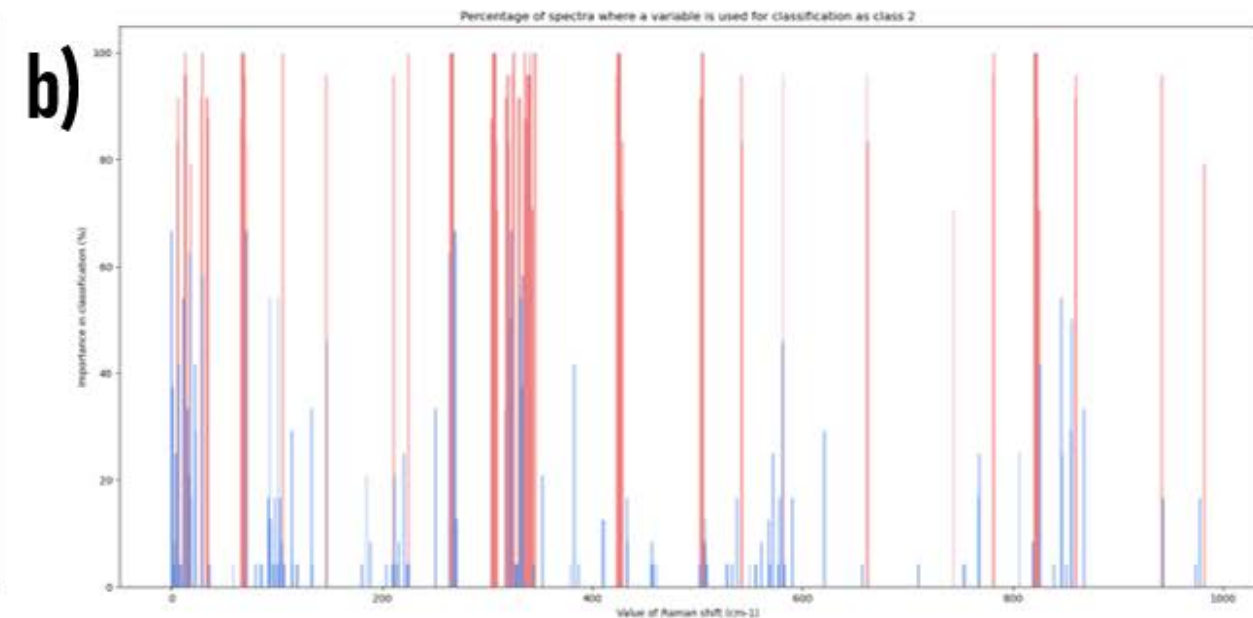
# **DISCUSSION**

# LACK OF GENERALIZATION

Hypothesis : Due to the Leave-One-Patient-Out Cross-Validation, there is no general important variable



Model trained over the 0th fold of the Leave-One-Patient-Out Cross-Validation.



Model trained over the 2th fold of the Leave-One-Patient-Out Cross-Validation.

**BOTH MODELS DO NOT AGREE ON WHICH ARE THE IMPORTANT VARIABLE !!!**

# **FUTURE WORKS**

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