



## ***“Understanding Predictions made by Machine Learning for Spectroscopic Atmospheric Characterisation”***

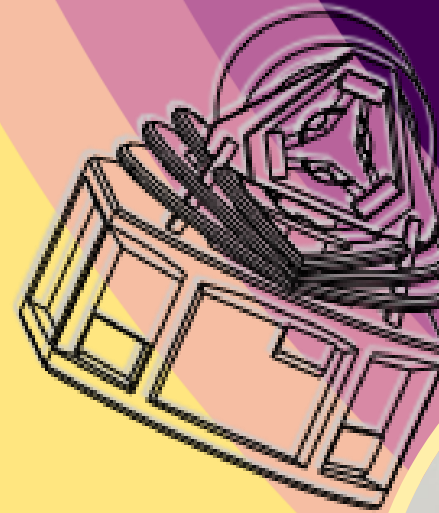
**Jools Clarke<sup>1</sup>, Gordon Yip<sup>2</sup>, and Nikos  
Nikolaou<sup>3</sup>**

<sup>1</sup> jools.clarke.23@ucl.ac.uk

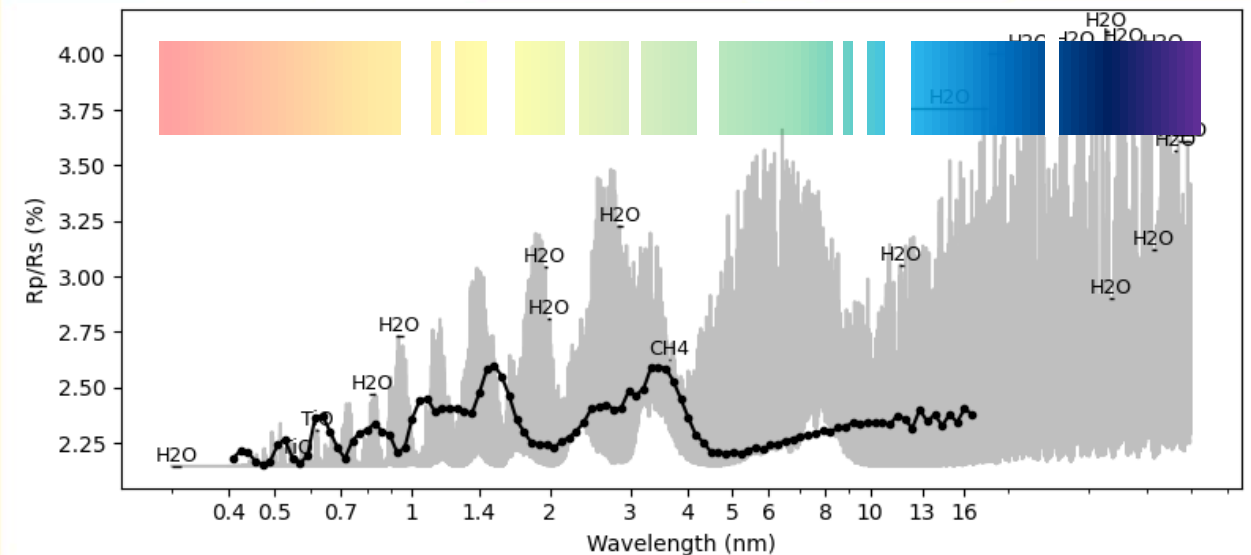
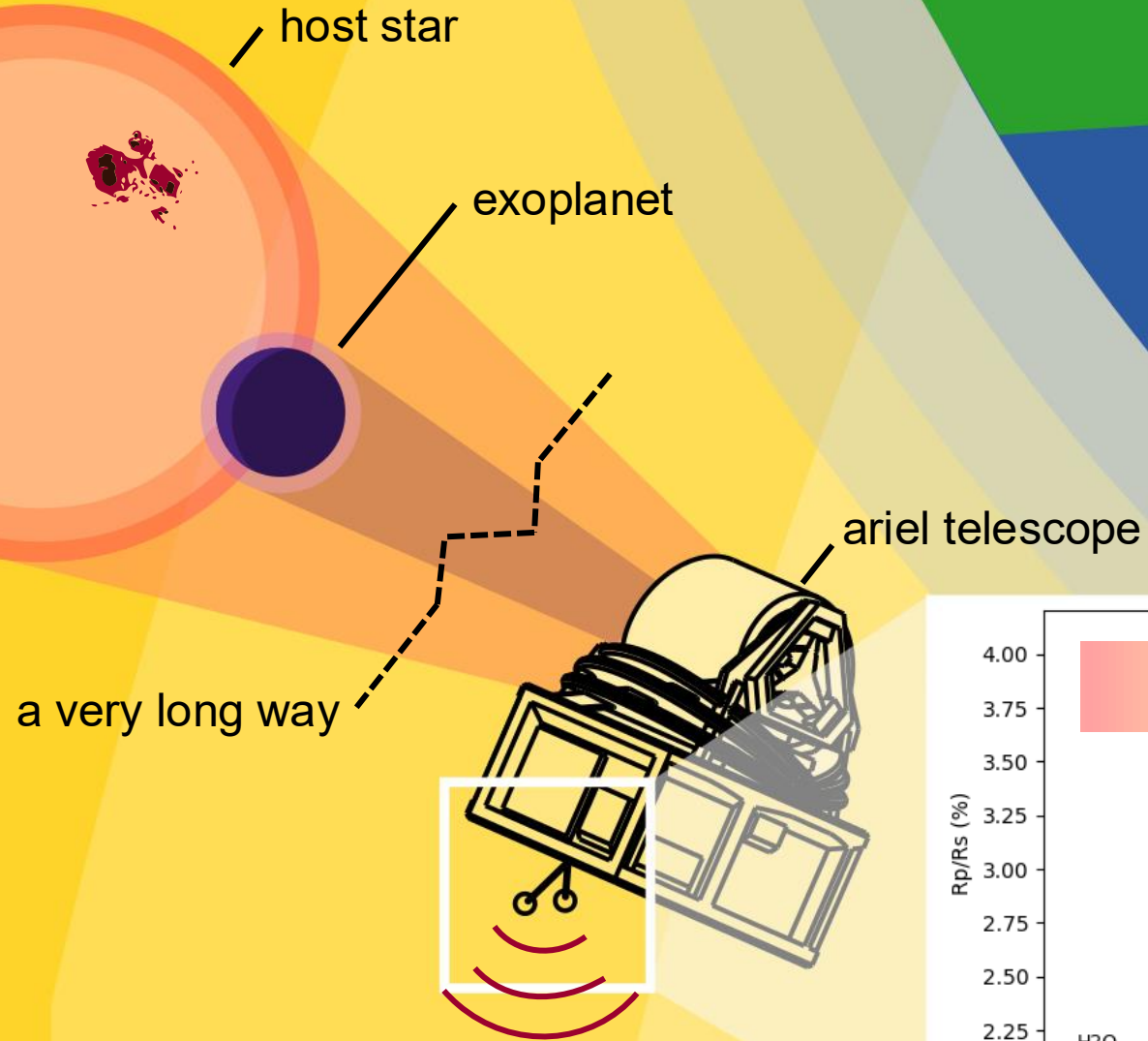
<sup>2</sup> kai.hou.yip@ucl.ac.uk

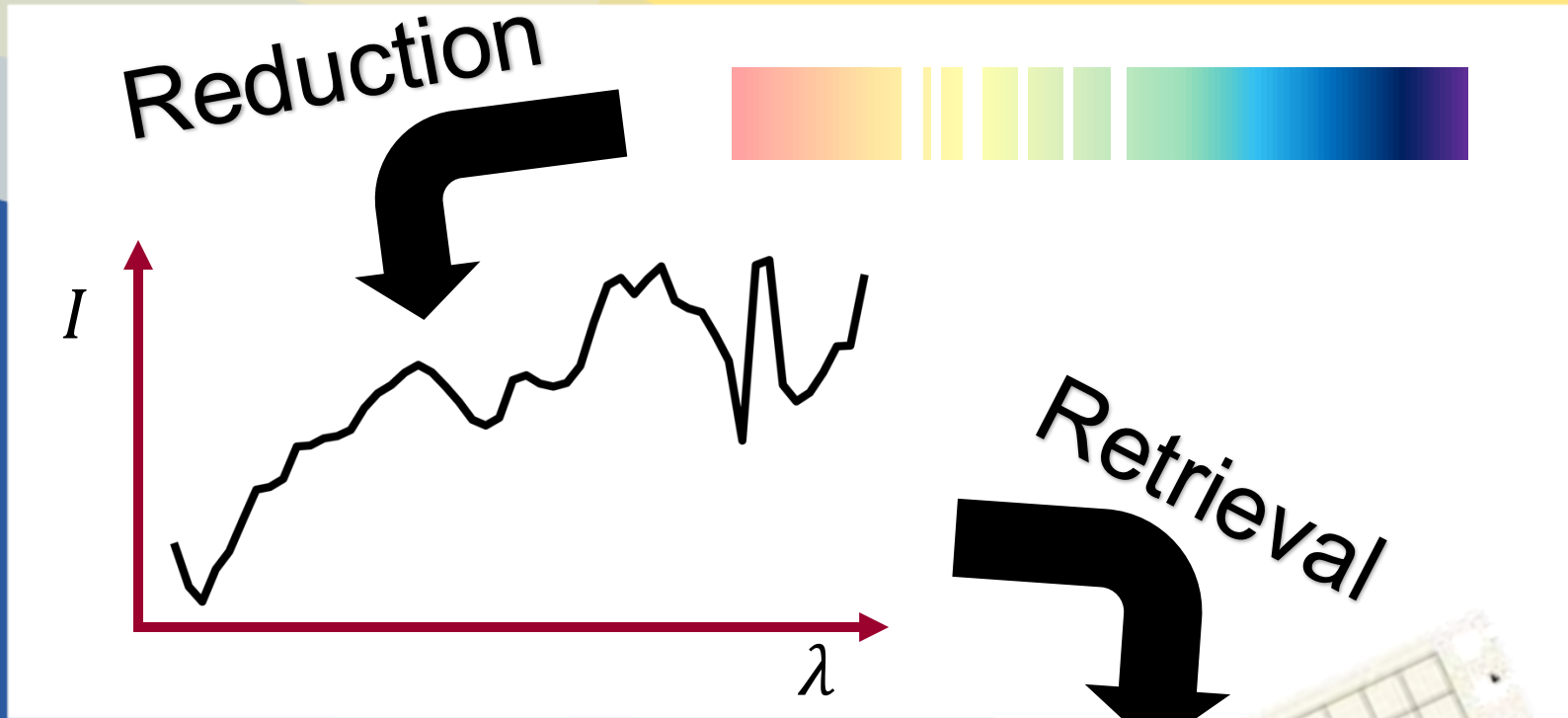
<sup>3</sup> n.nikolaou@ucl.ac.uk

*With thanks to Sushuang Ma for the data*



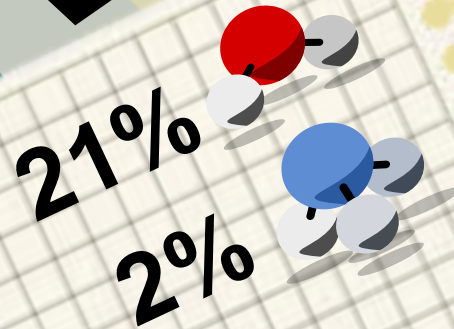
# Transit Spectroscopy: a very quick recap!

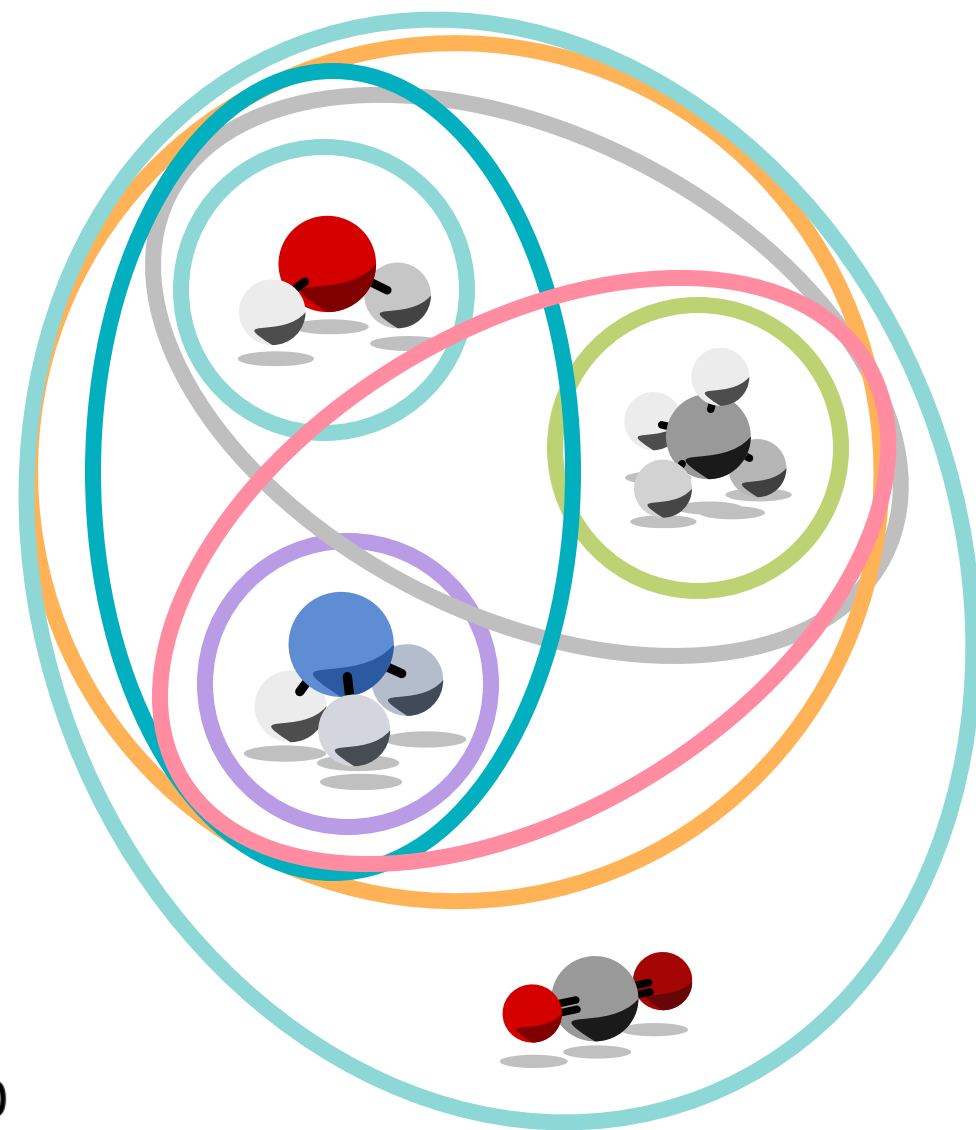
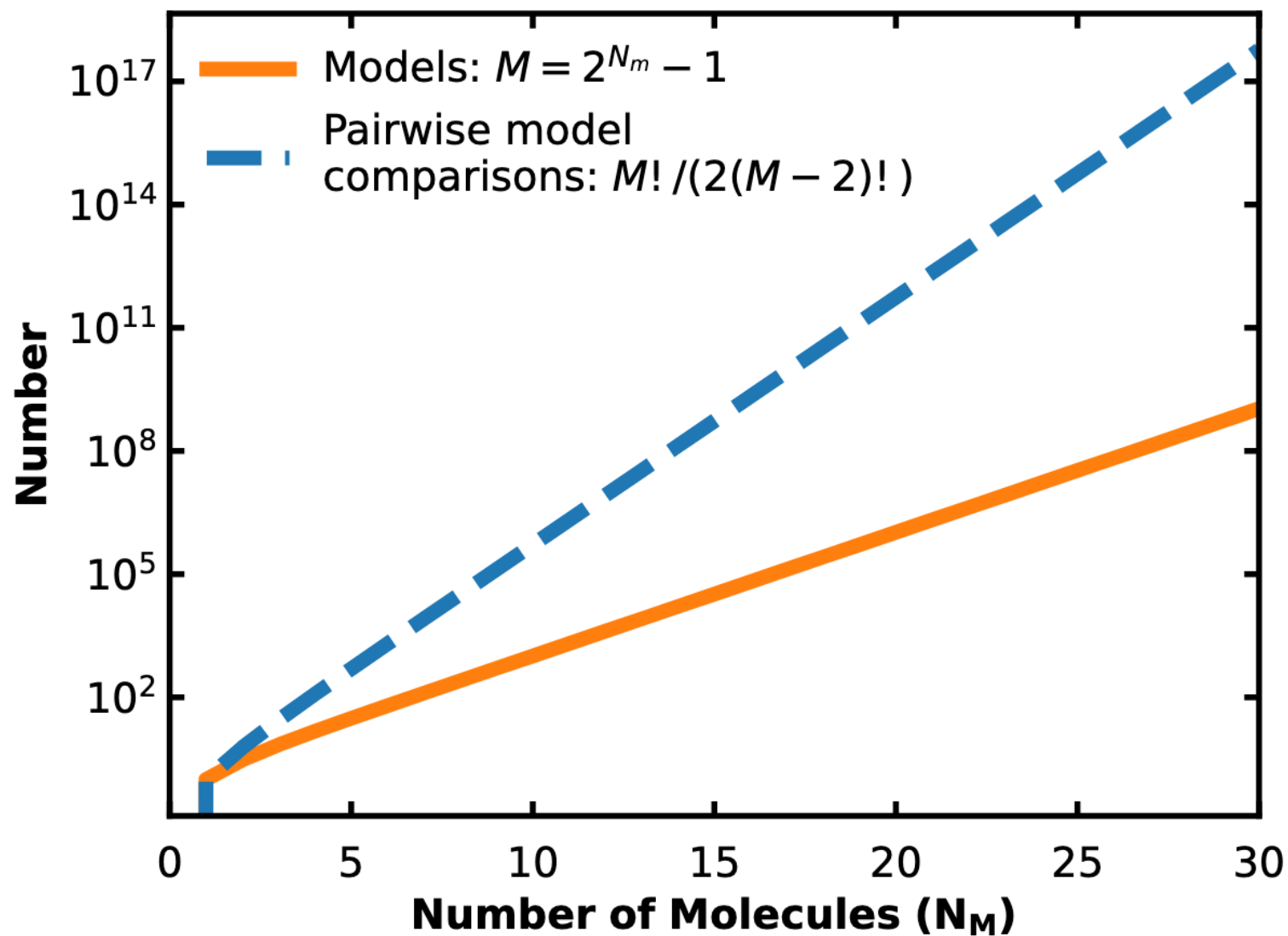




Forward Model

21%  
2%





(Welbanks *et al.*, 2025)

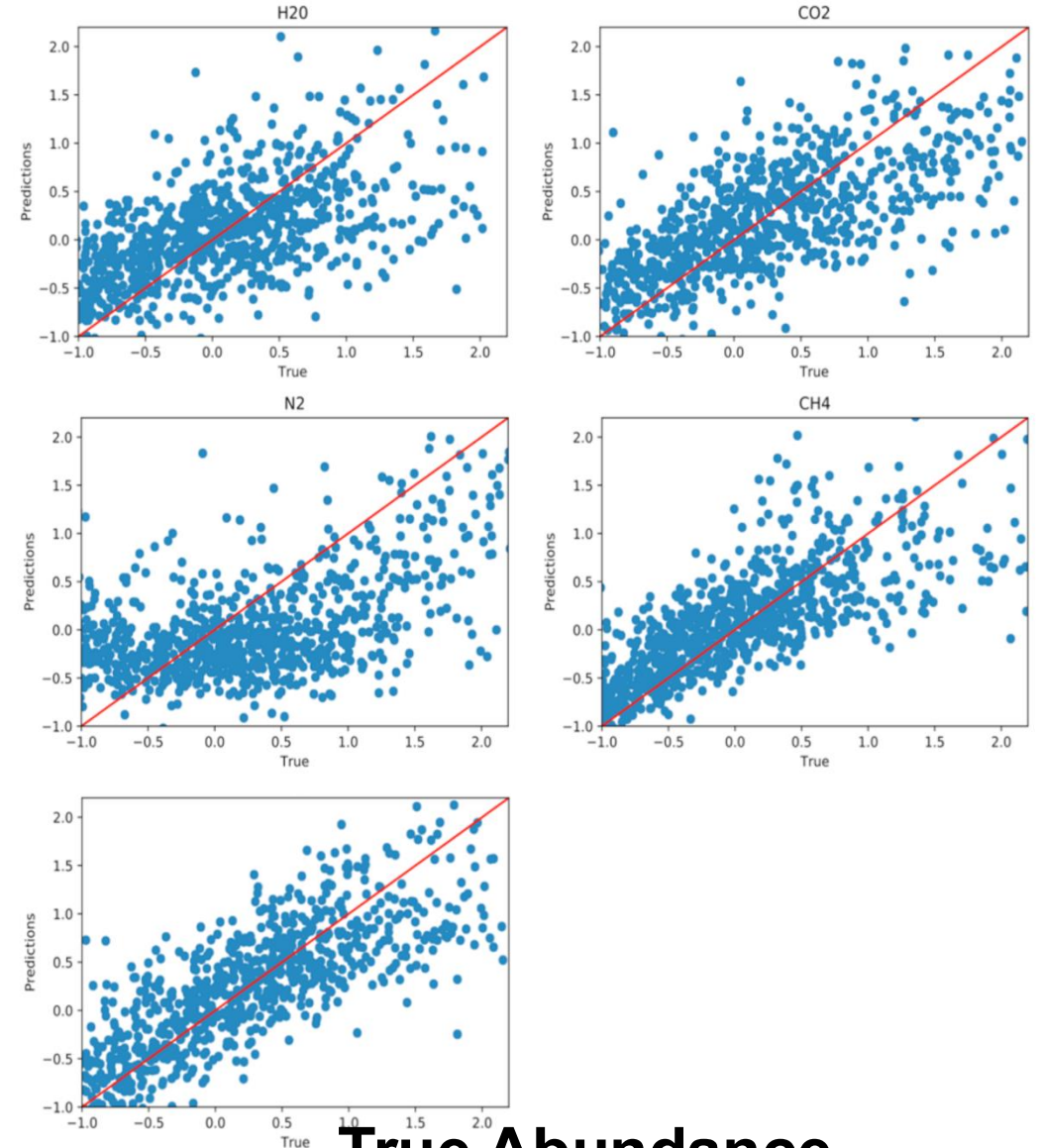
## INARA

**Comprehensive grid search**  
over model architectures and  
hyperparameters

Established **1D CNNs** as best  
model architecture

Significantly **accelerated**  
compared to traditional  
Bayesian retrievals

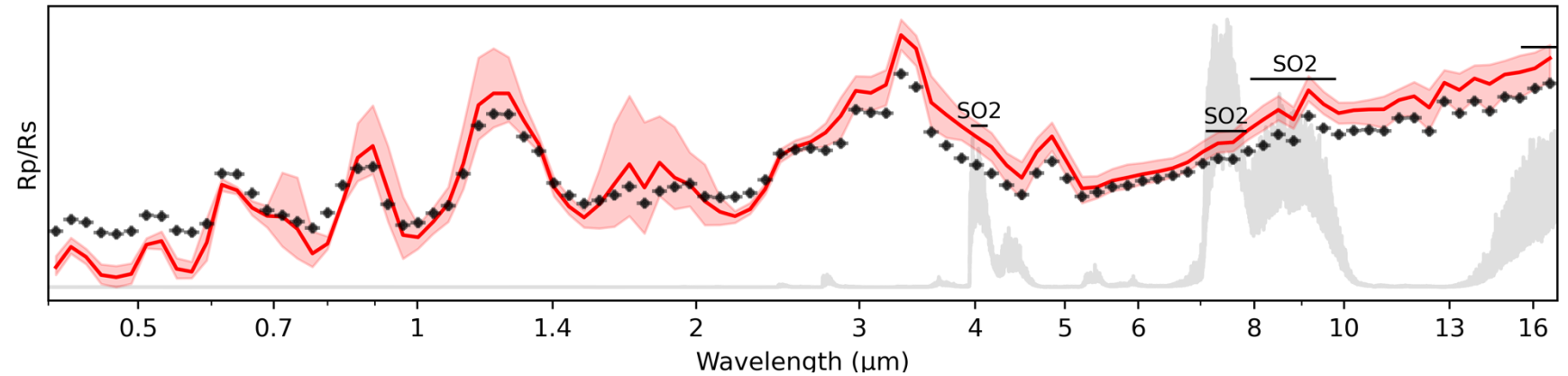
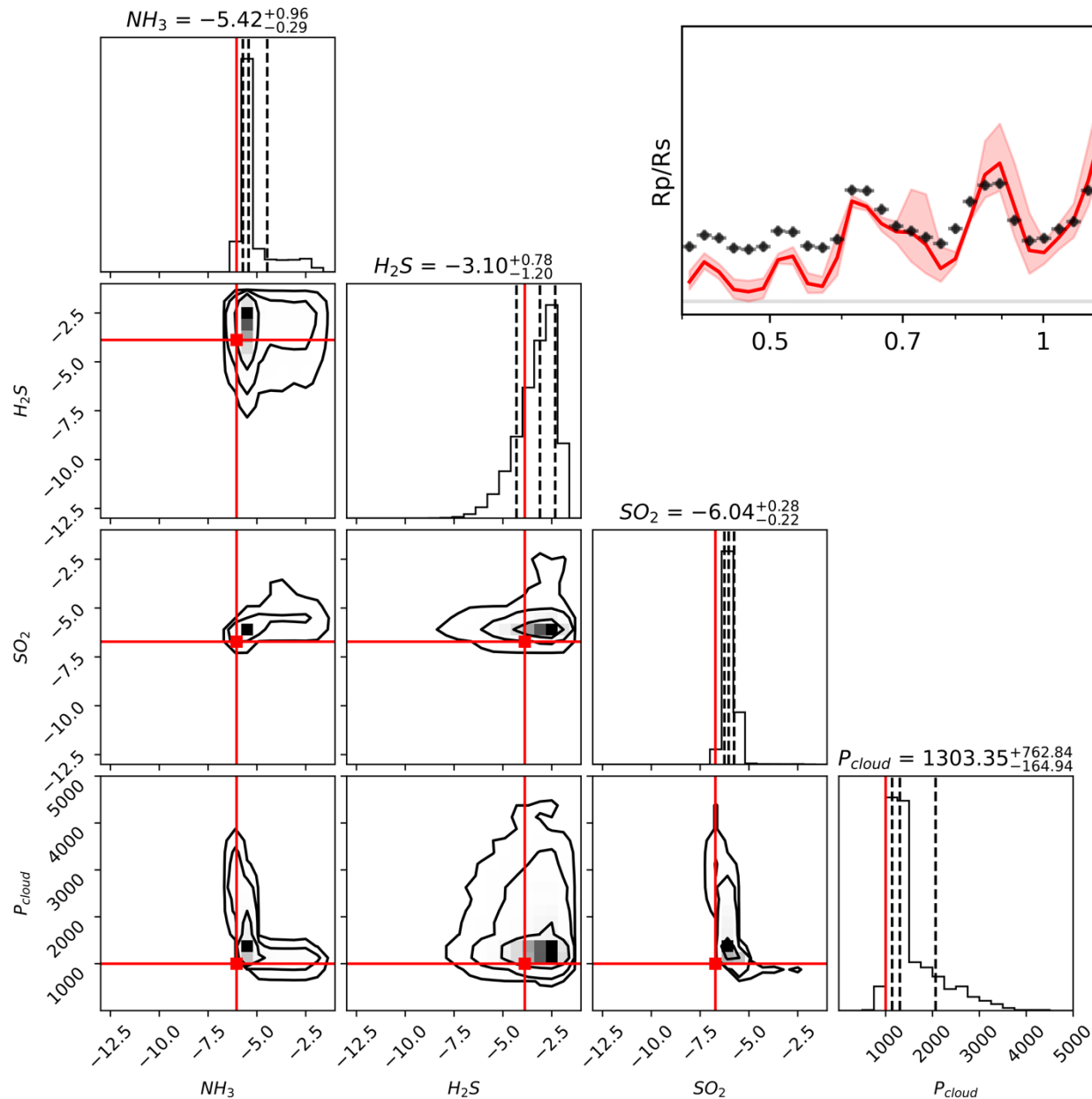
Prediction



**True Abundance**

(Soboczenski *et al.*, 2018)

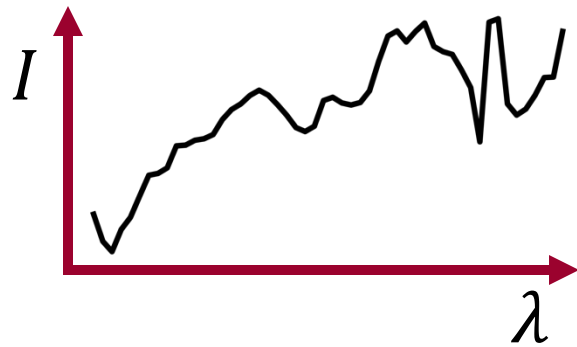




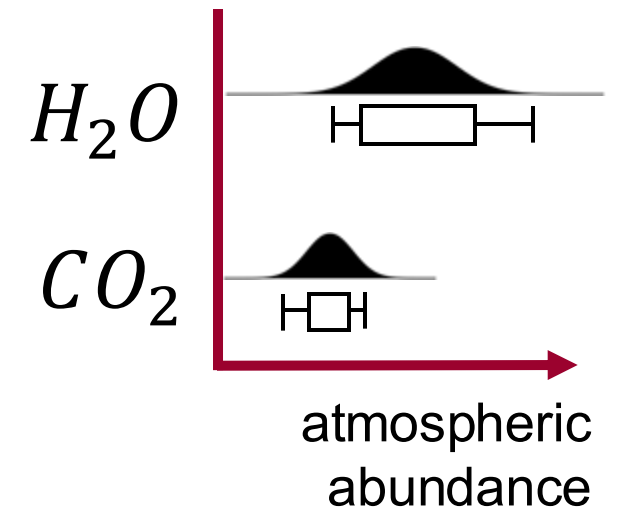
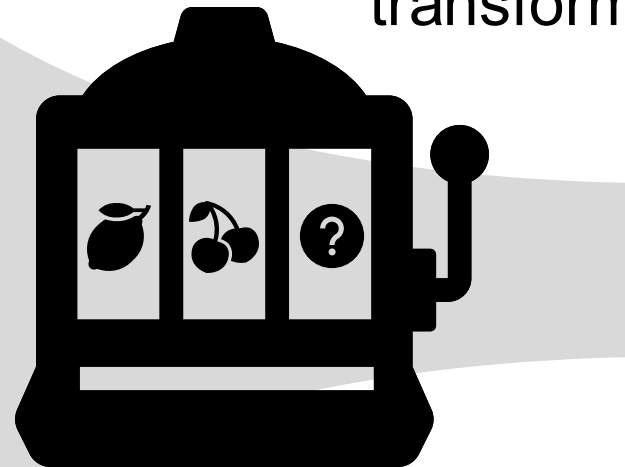
## PERTURB

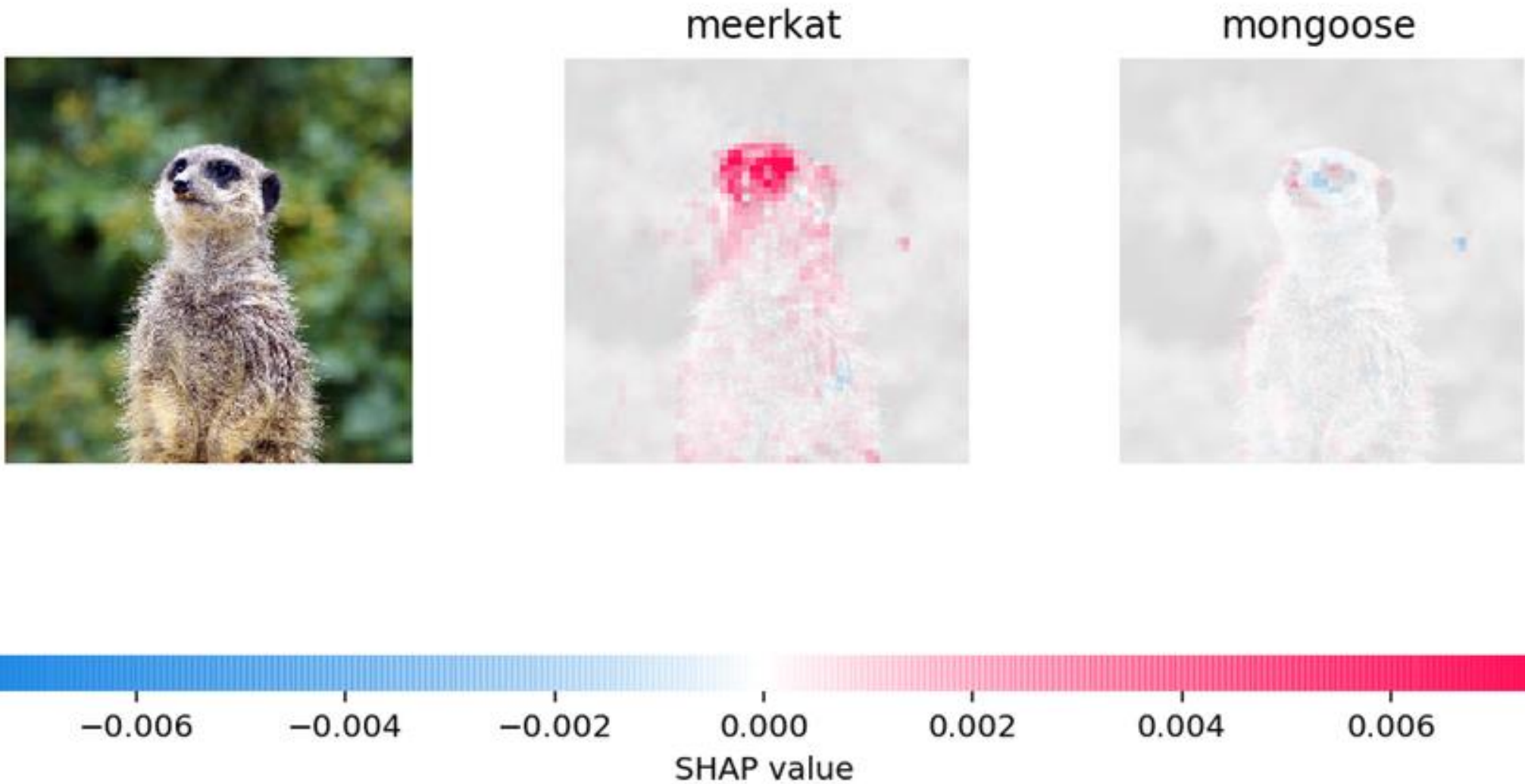
**Accuracy** of these retrievals  
 on simulated data is  
**sufficient** for making useful  
 statements about a system

(Clarke *et al.*, in prep.)



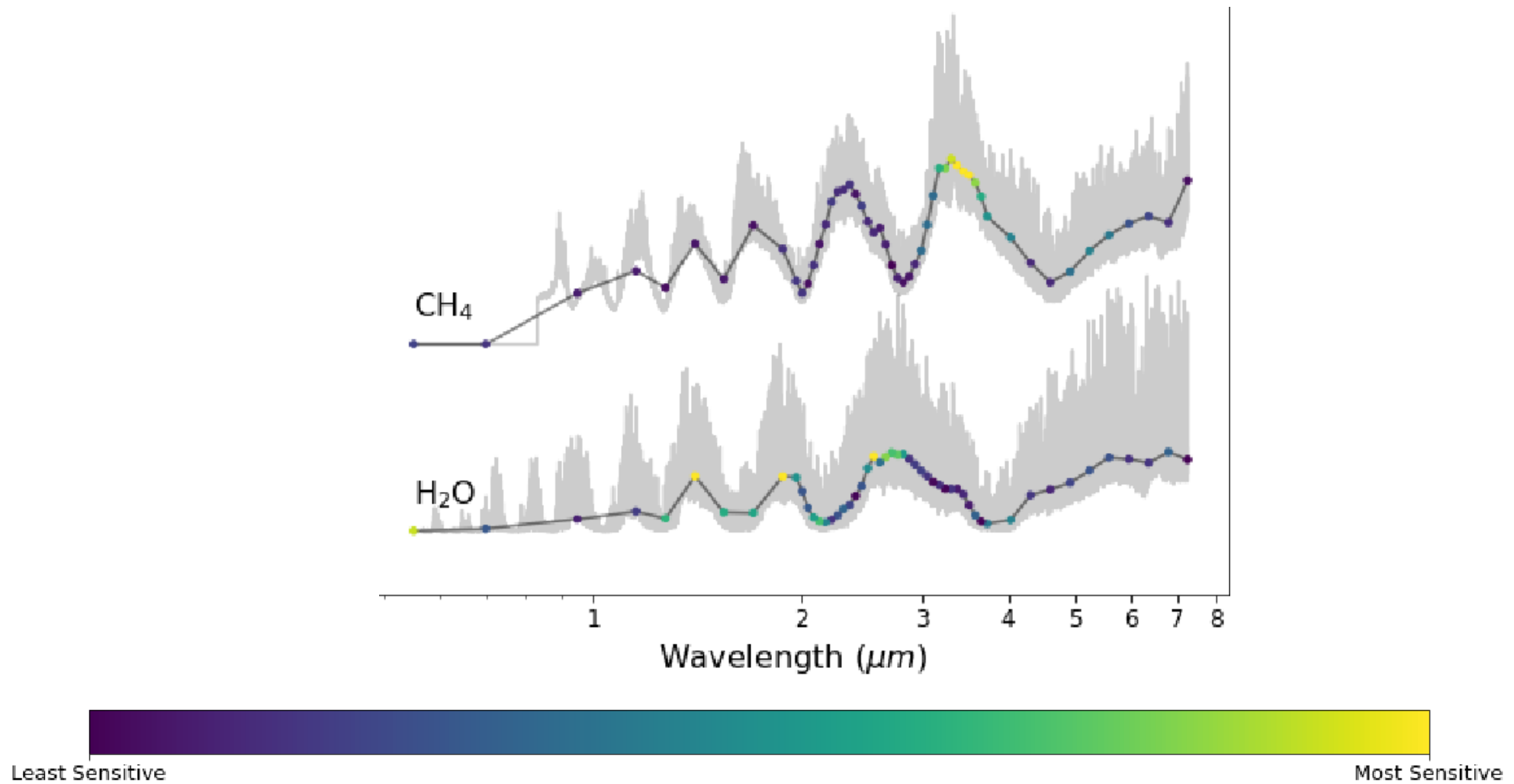
Set of **non-linear** matrix transformations



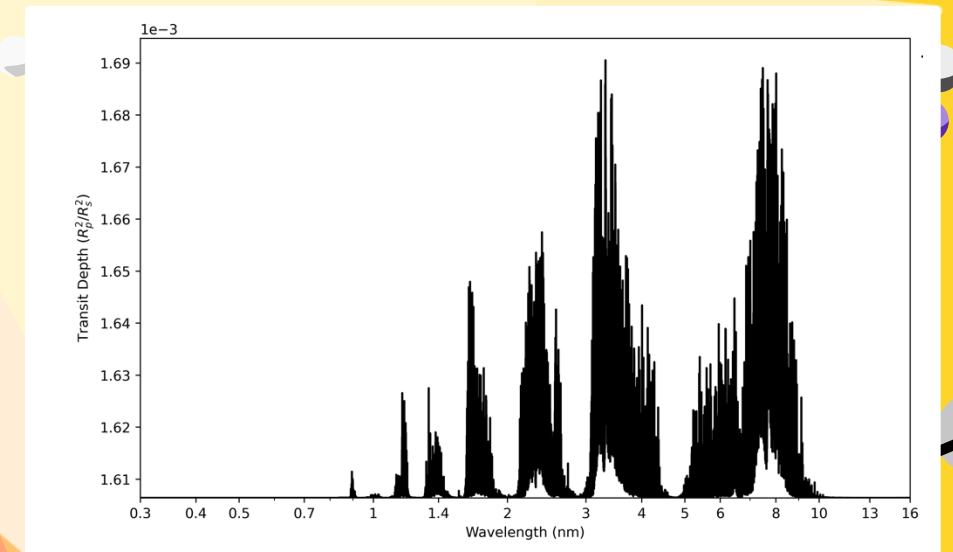
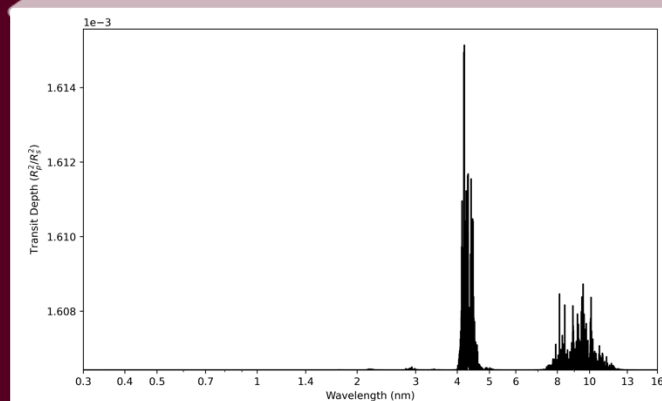
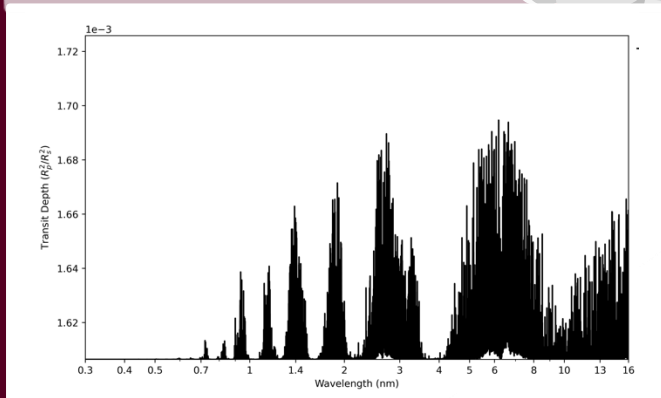
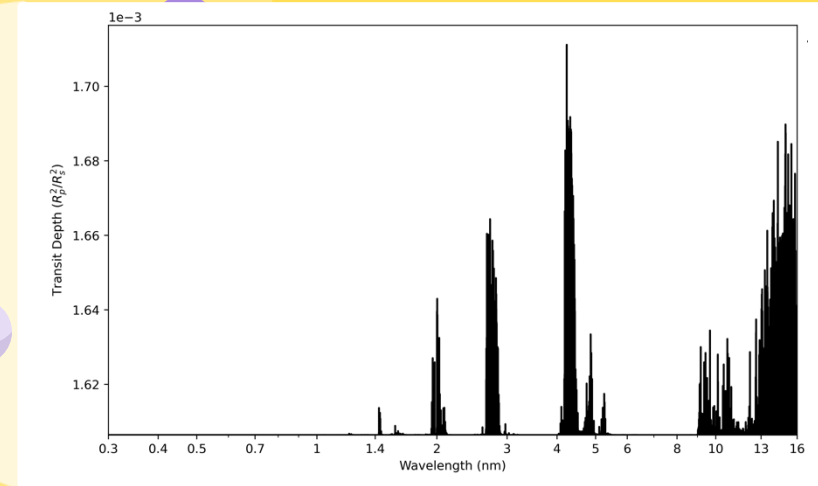
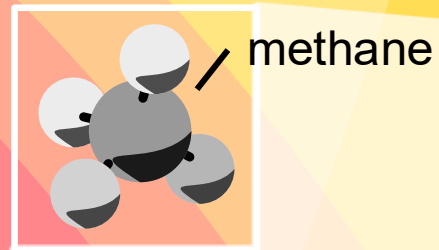
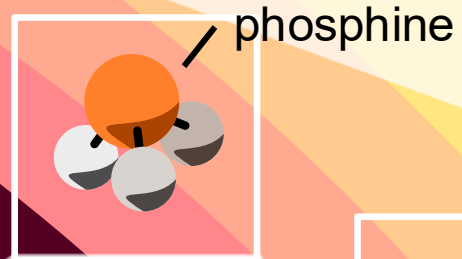
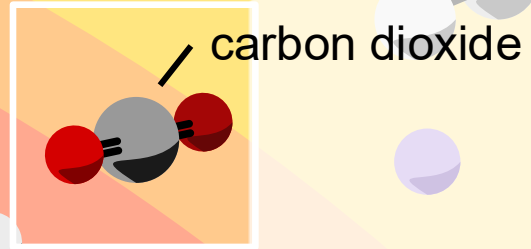
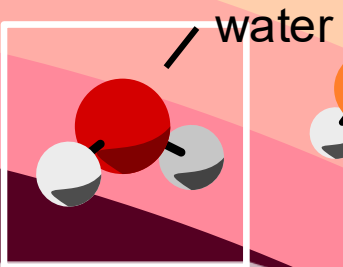


SHAP paper: (Lundberg and Lee, 2017), image: (Shojaeinasab *et al.*, 2024)





(Yip *et al.*, 2021)



## Introducing



**P** hysical  
**E** xplainability  
**R** anking  
**T** echniques for  
**U** nderstanding  
**R** etrieval  
**B** lack-boxes

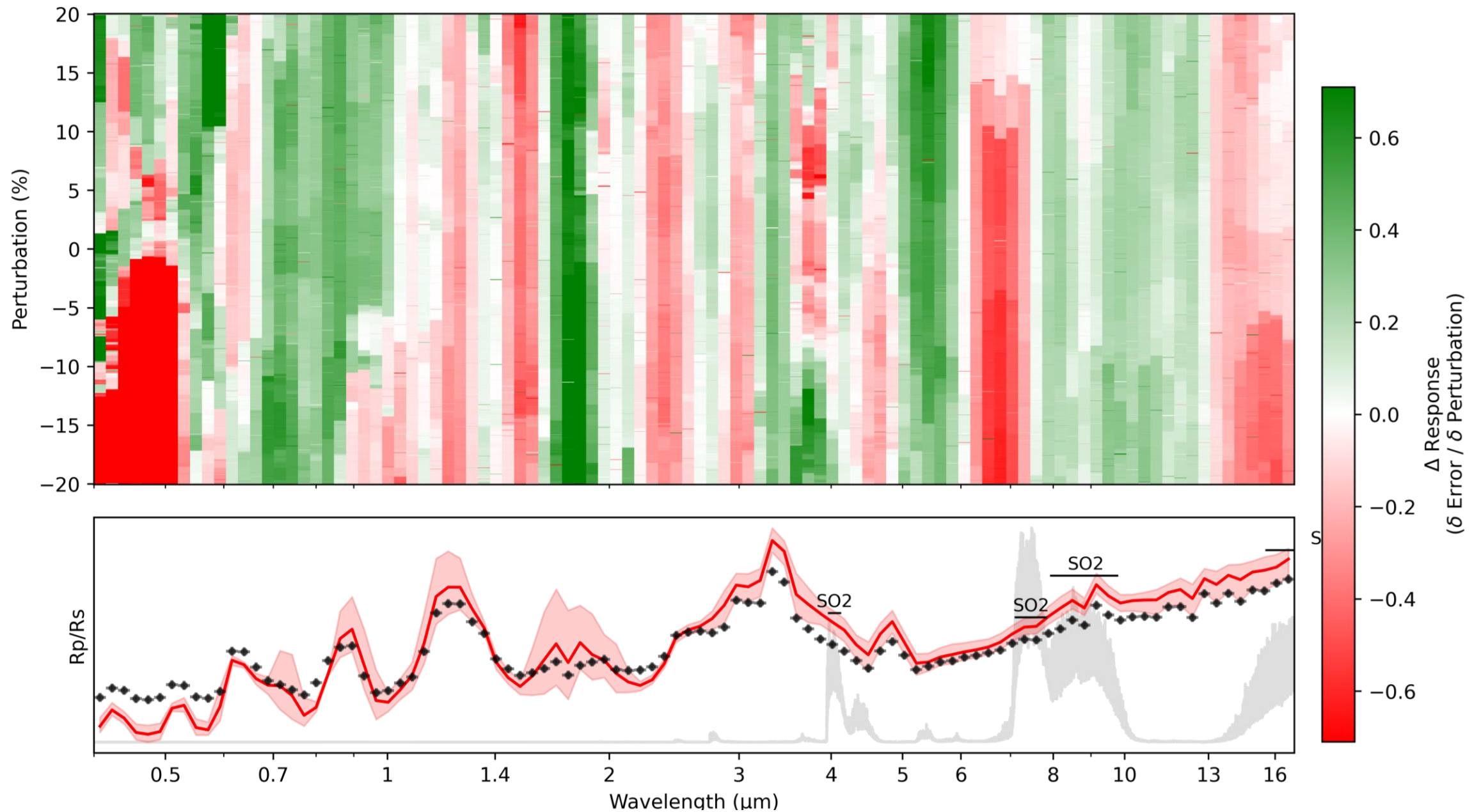
A new **lightweight** method for ML retrieval model interpretability based on **noise injection** and **response regression**.

Built to be **modular** and **tunable**

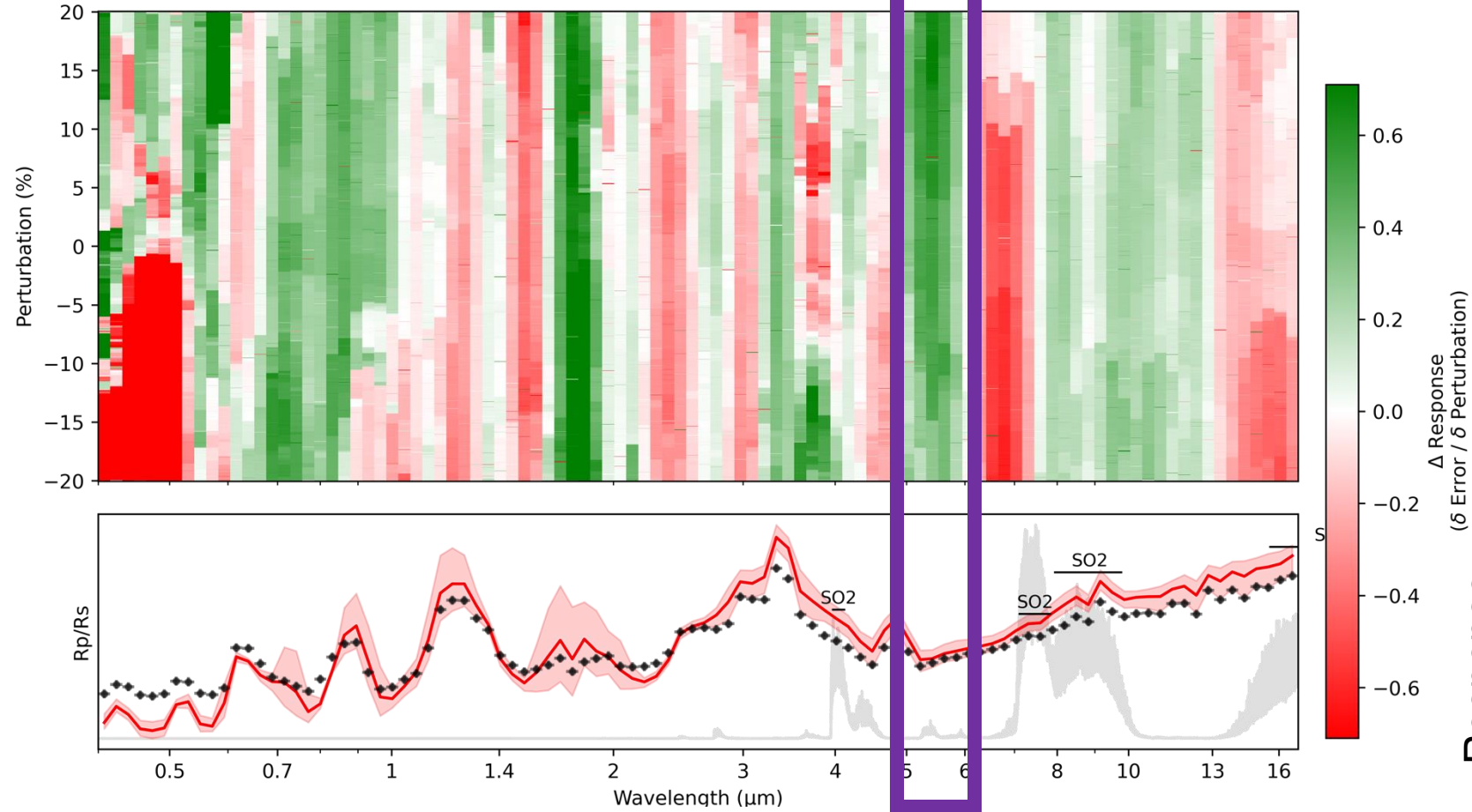
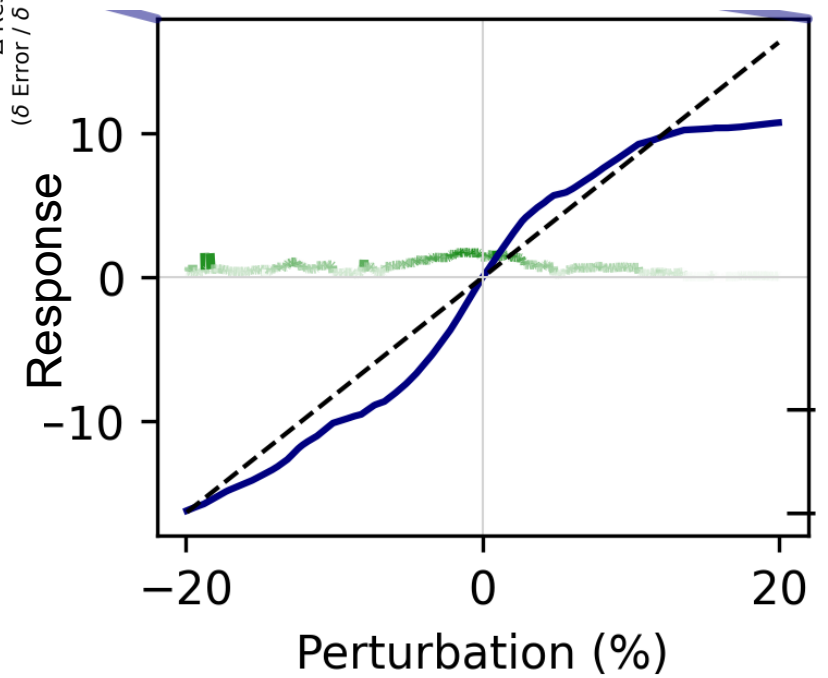
**Model agnostic**, can be applied to any retrieval methodology

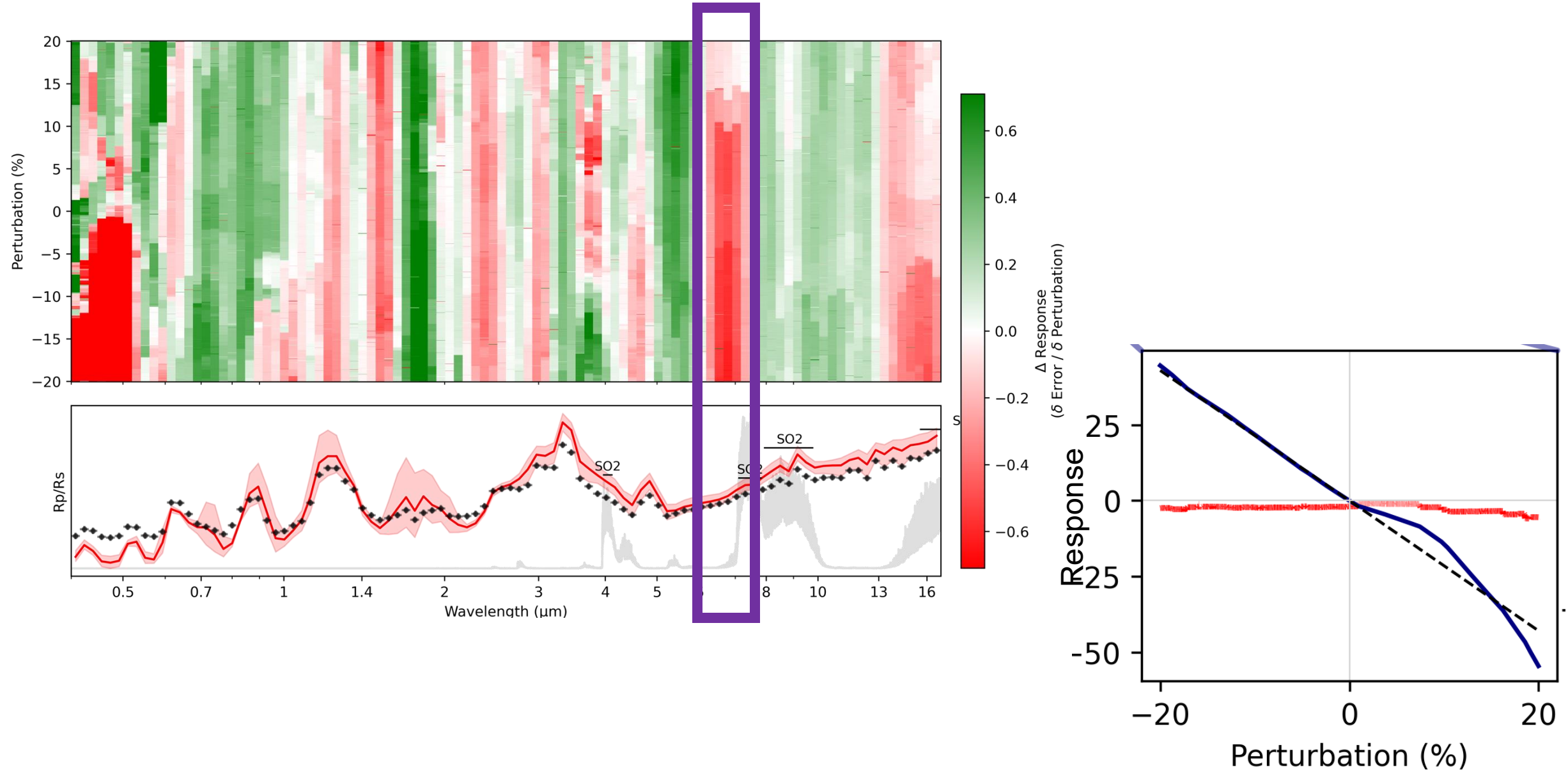
(Clarke *et al.*, in prep.)

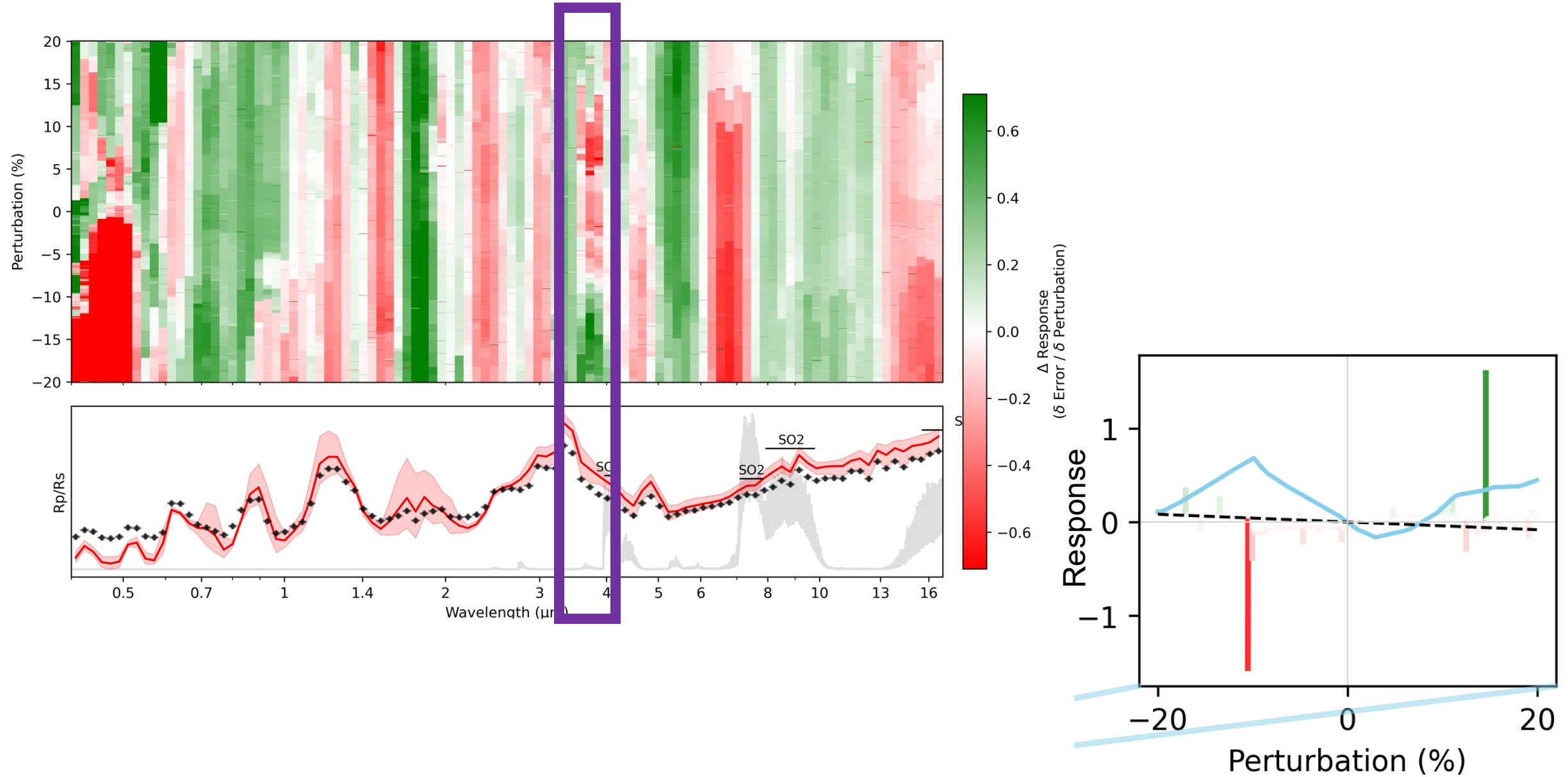






 $\Delta \text{Response}$   
( $\delta \text{ Error} / \delta \text{ Perturbation}$ )





**Help shape PERTURB for your  
research! Fill out the survey**

**or read more about the project**



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**publication in prep.**

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