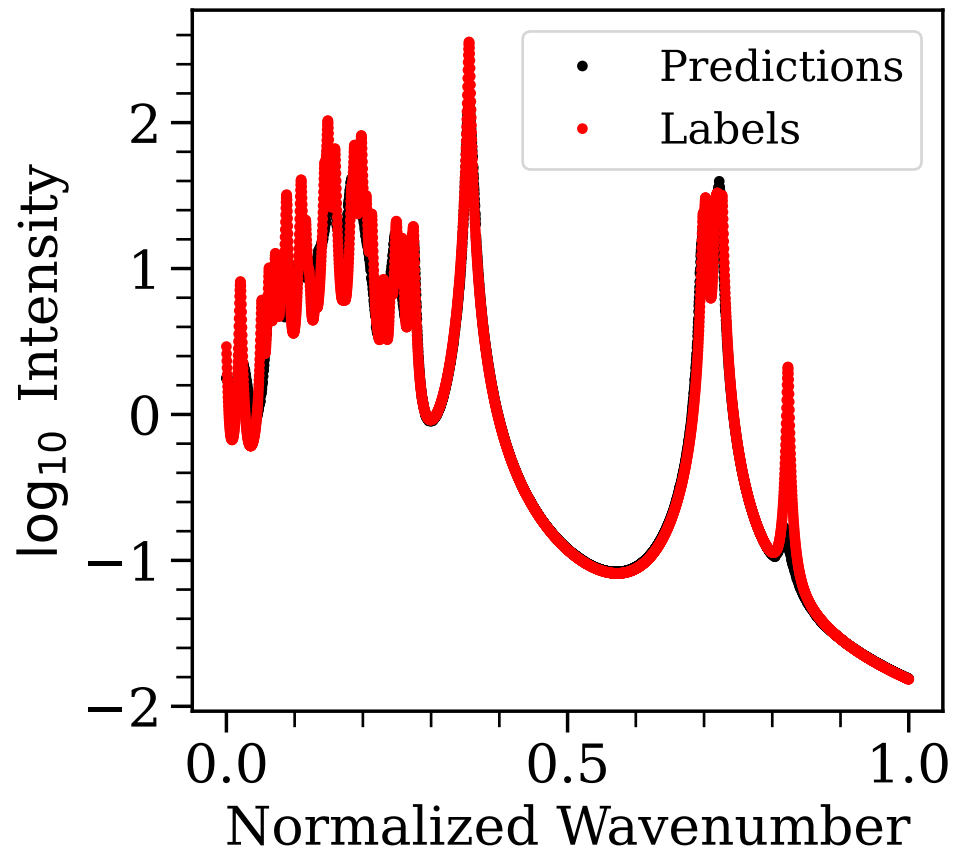## CC1C2NC2COC1=O

CC1C2NC2COC1=O

Left panel — log₁₀ Intensity vs Normalized Wavenumber:
- Predictions (black)
- Labels (red)

Right panel — Uncertainty vs Normalized Wavenumber:
- Aleatoric Uncertainty (blue)
- Epistemic Uncertainty (green)