Standoff Detection of Chemical Residues using Quantum Cascade Lasers

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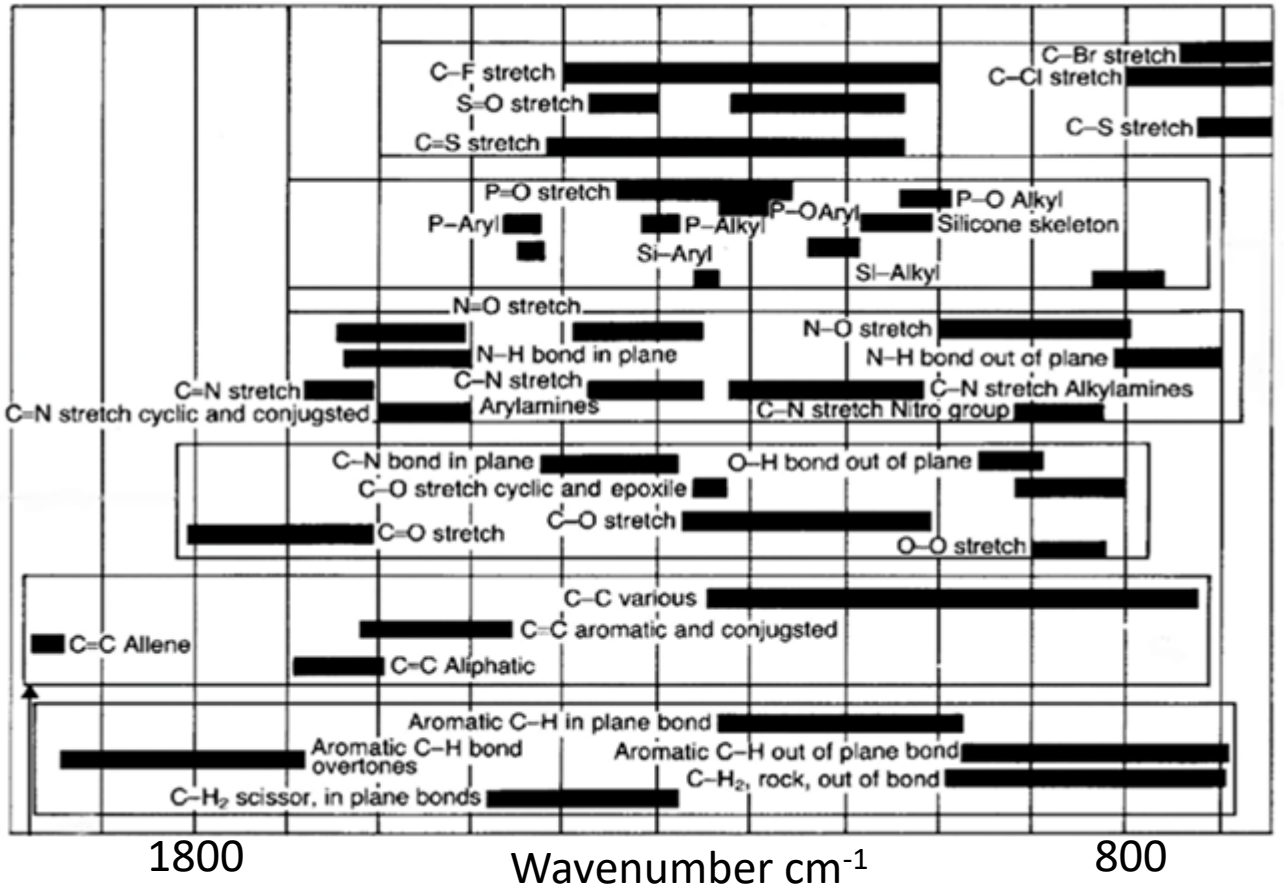
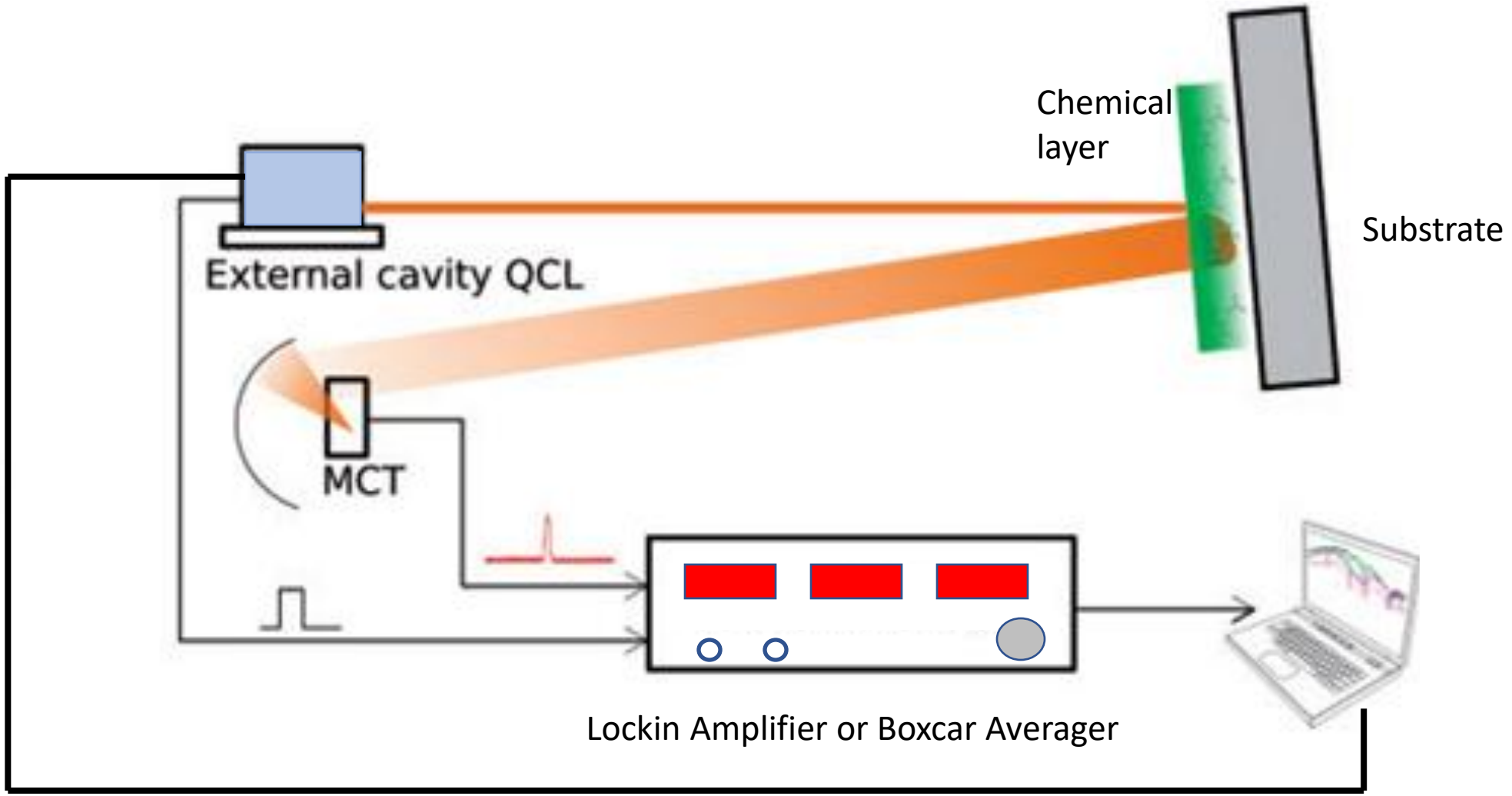
- Coverage of the fingerprint range
- QCLs are bright, collimated, wavelength tunable
- Standoff demo with our lasers

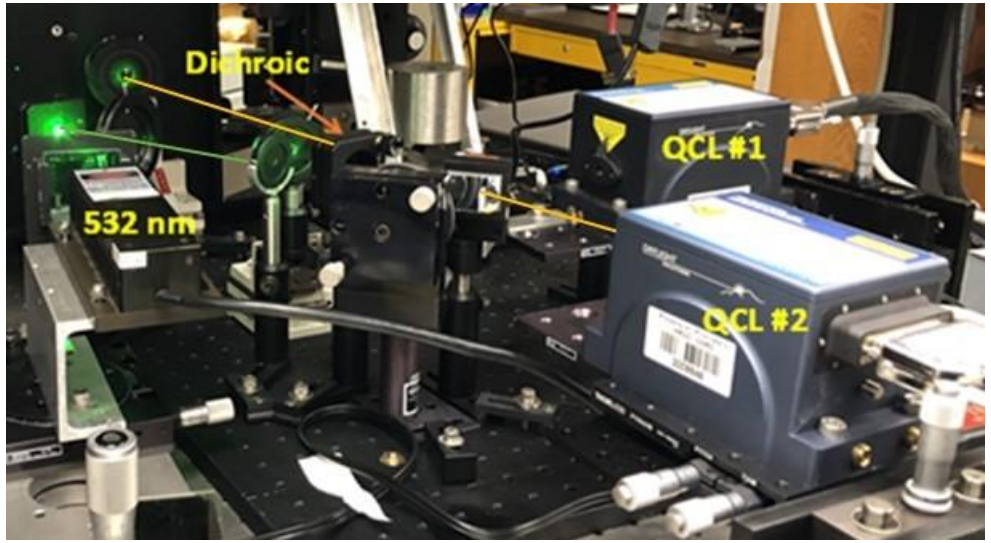


Standoff detection of chemical residues using quantum cascade lasers

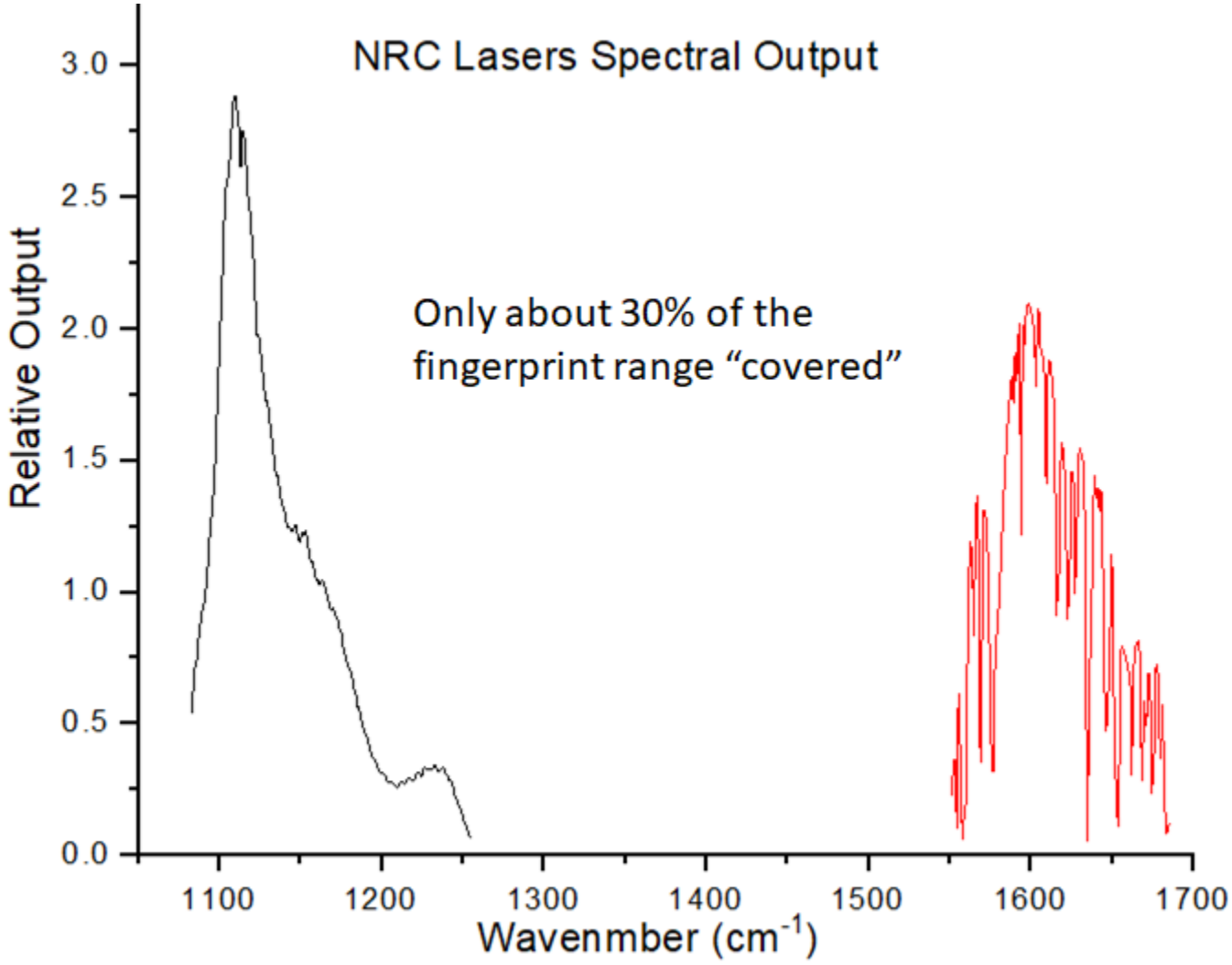


Quantum Cascade Lasers – Spectra

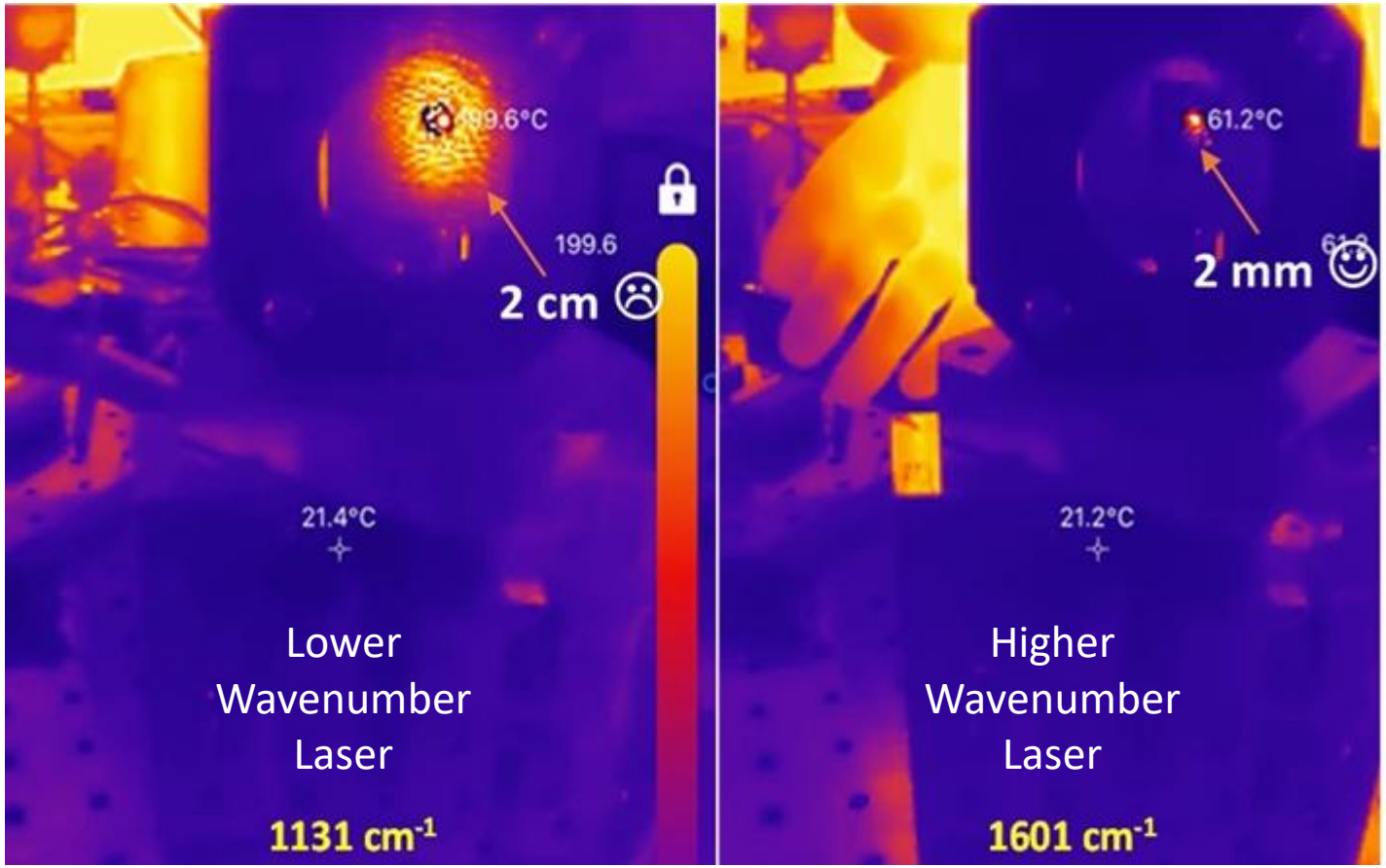
The Daylight Solutions QCLs



For alignment, the QCLs have a common path with a 532 nm laser

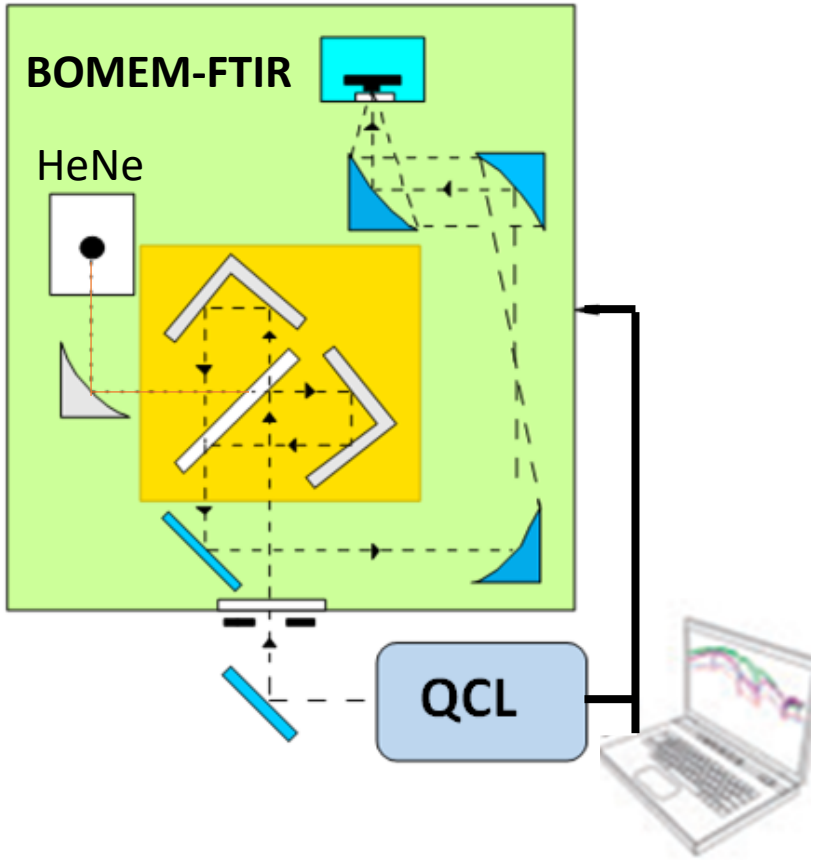


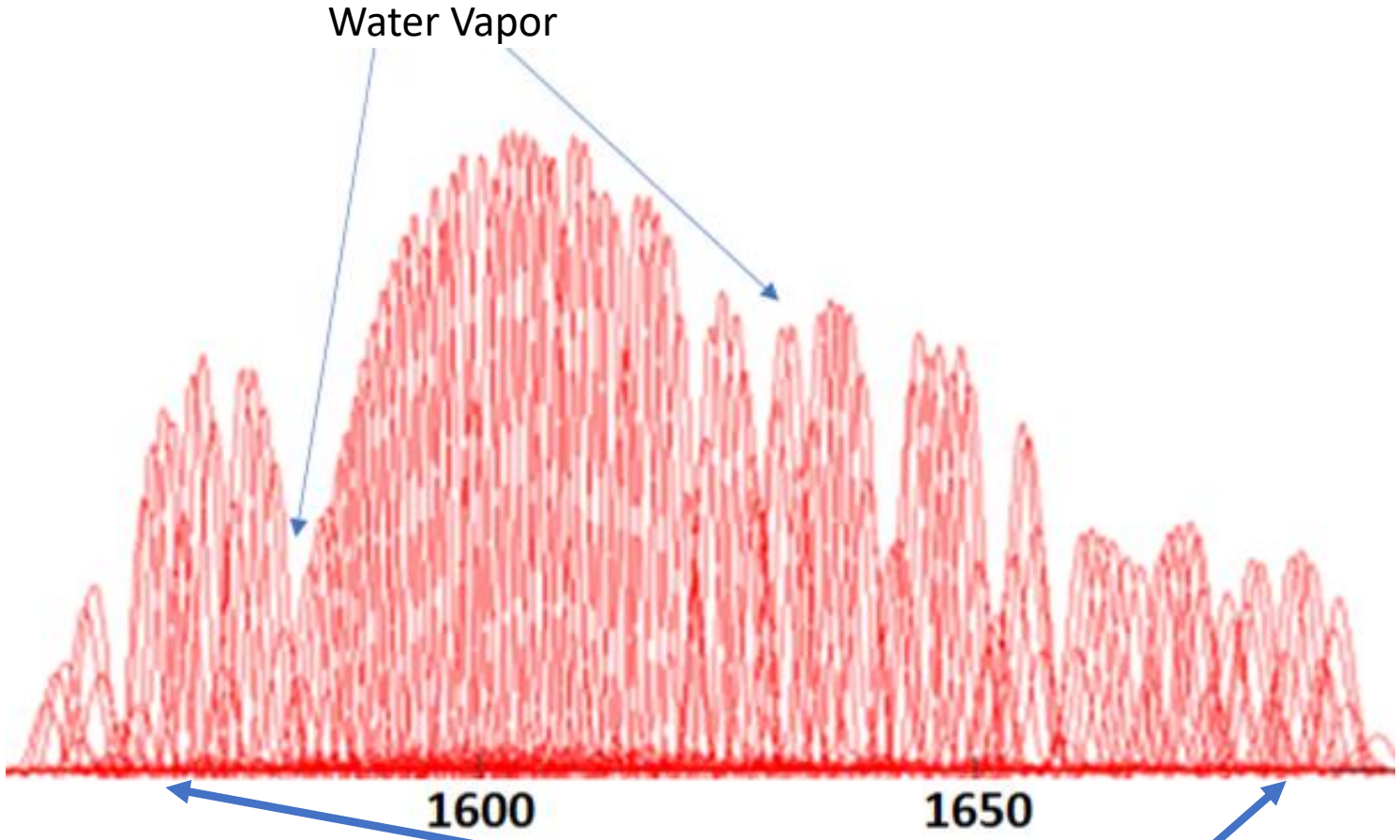
QCL Characteristics: Beam size, Collimation



Thermal images ~ 1 meter from the lasers

Measuring QCL Spectrum: Wavenumber Calibration 1550 – 1685 cm^{-1}

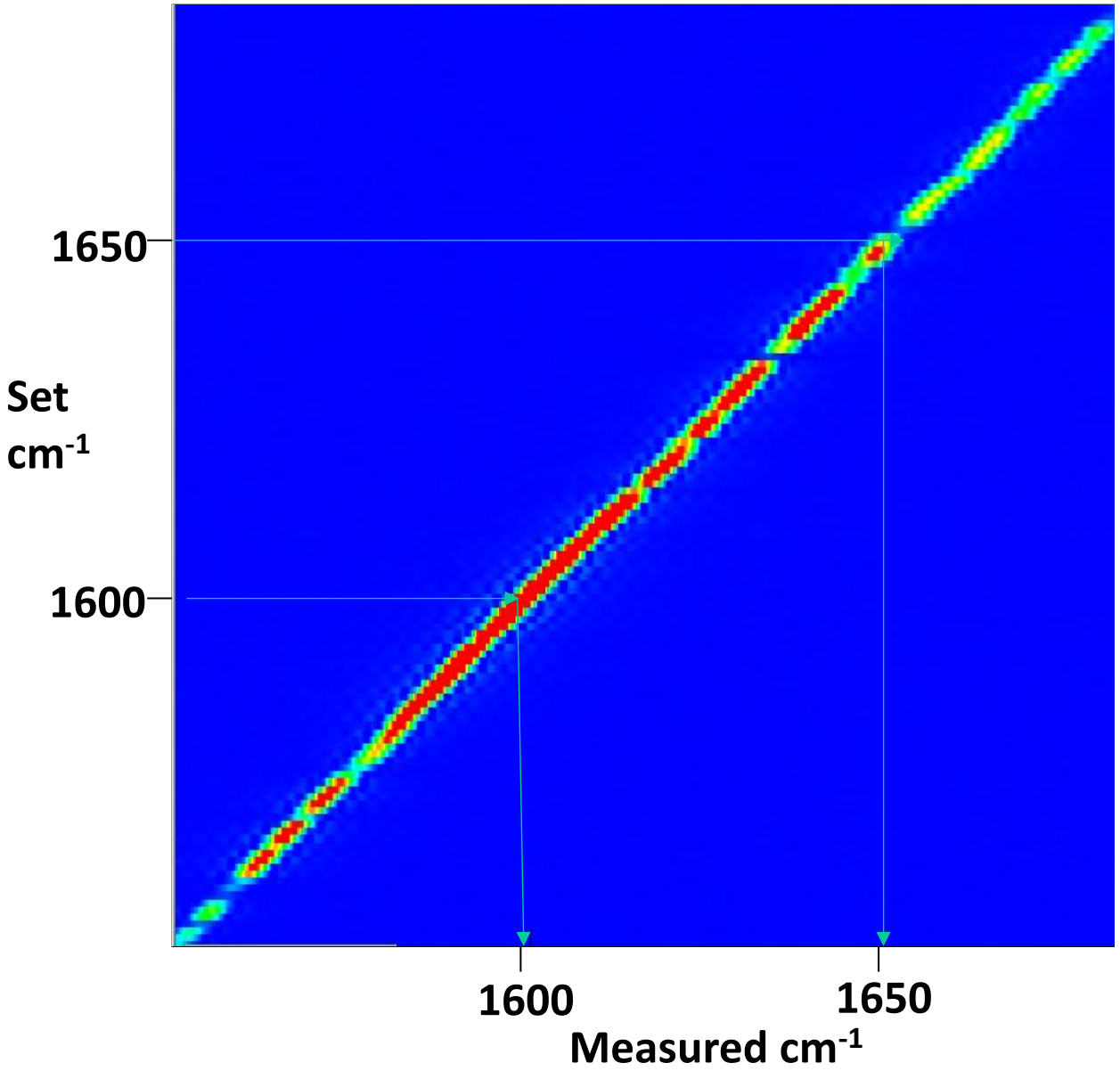


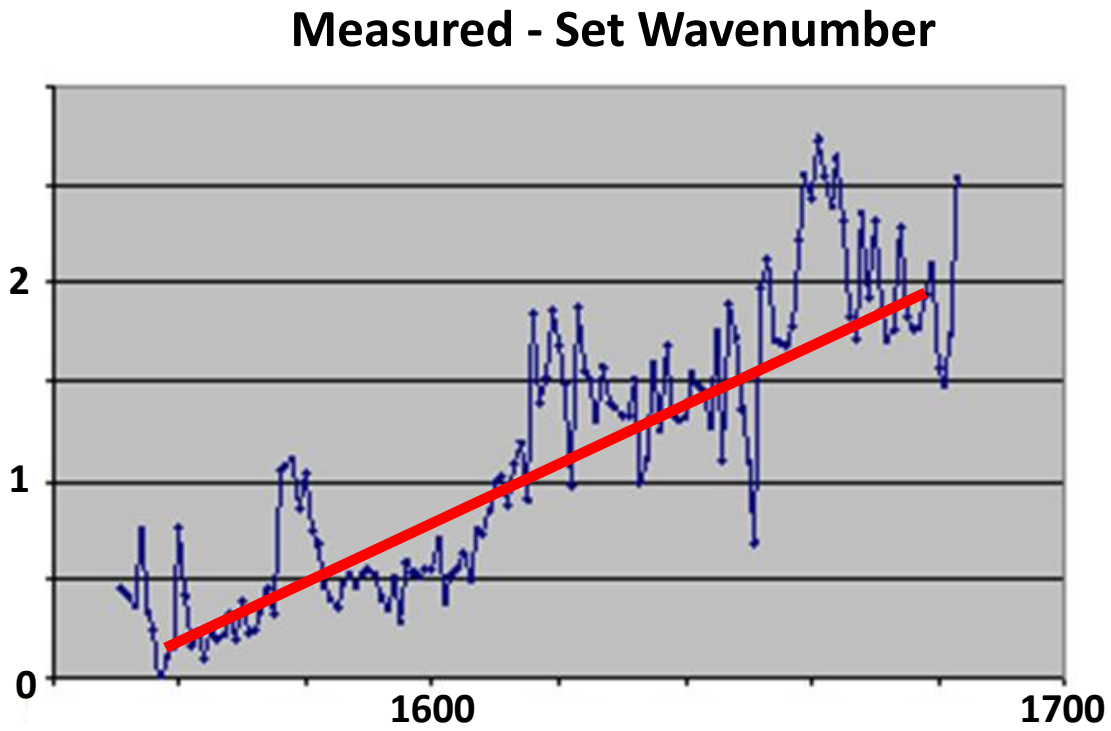


133 individual specta superimposed

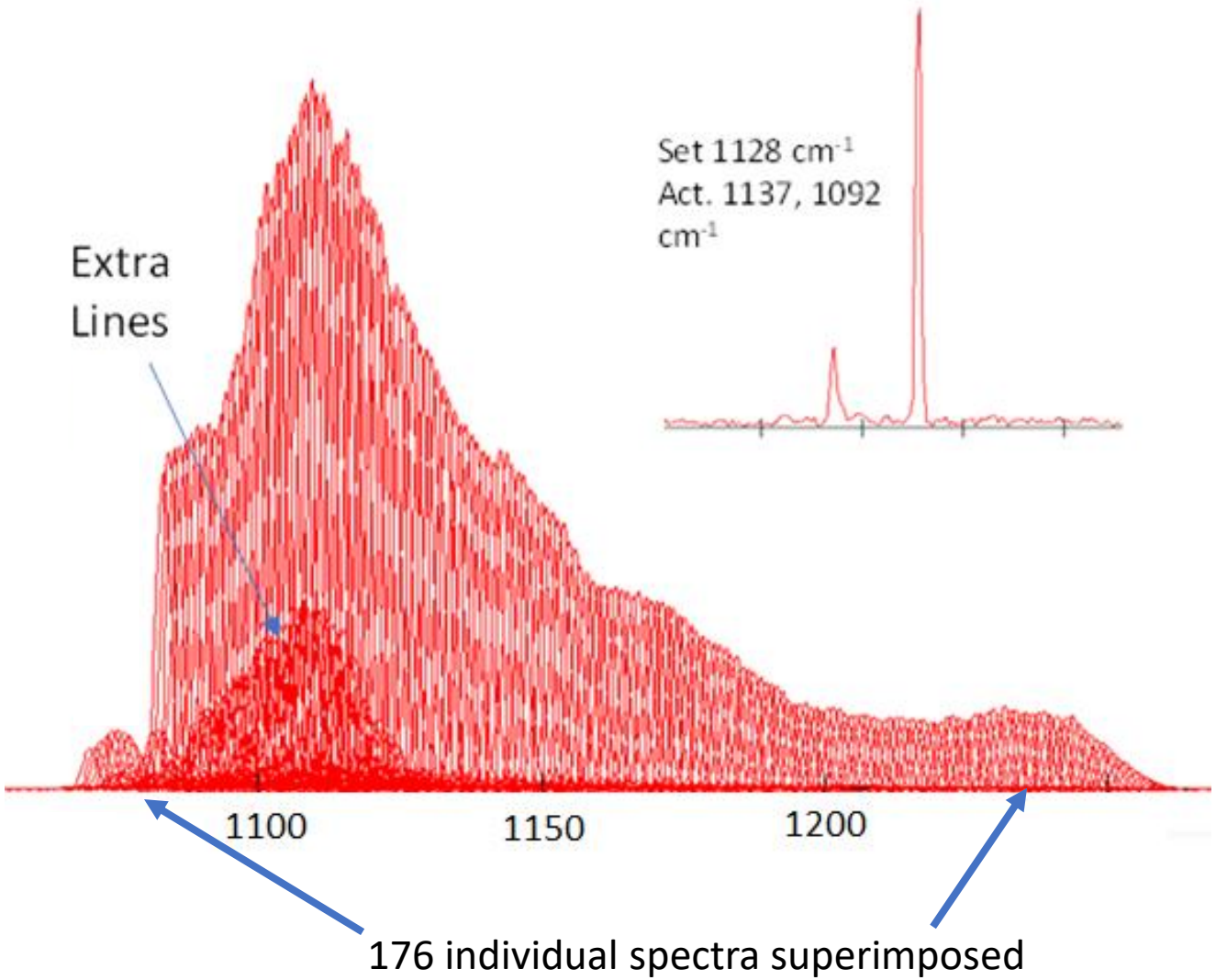
Bomem MB FTIR as a wavemeter using its external port. Spectra every 1 cm^{-1}
Measurement Program: step QCL cm^{-1}, save interferogram/HeNe fringes, repeat next step (+1 cm^{-1}), analyze interferogram files into spectra

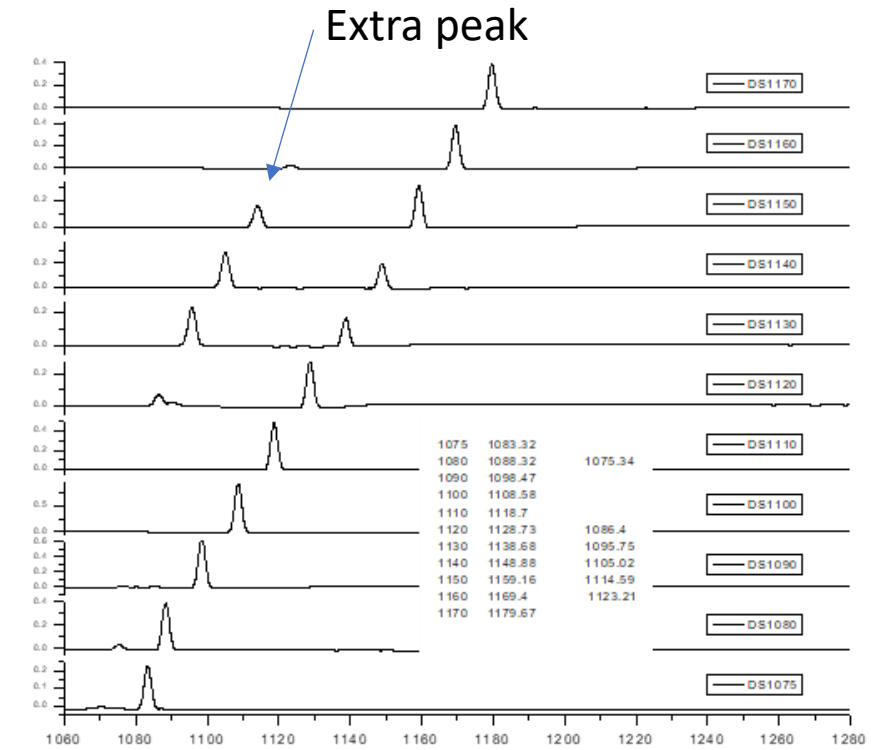
For spectroscopy: need the actual wavenumber value for a given setting

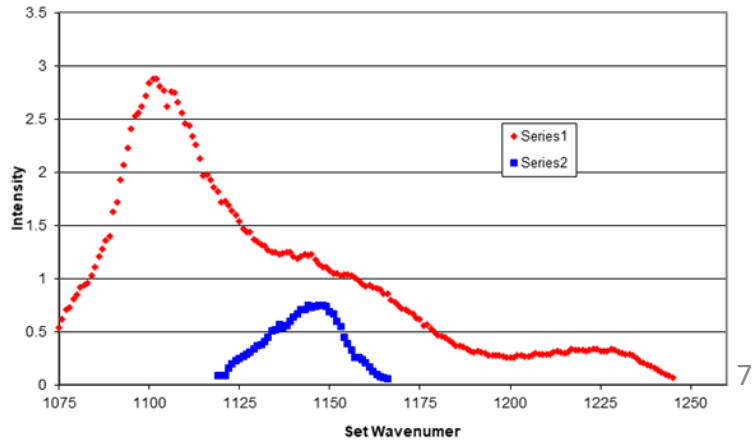




QCL Spectrum? Wavenumber Calibration 1075 – 1250 cm^{-1}



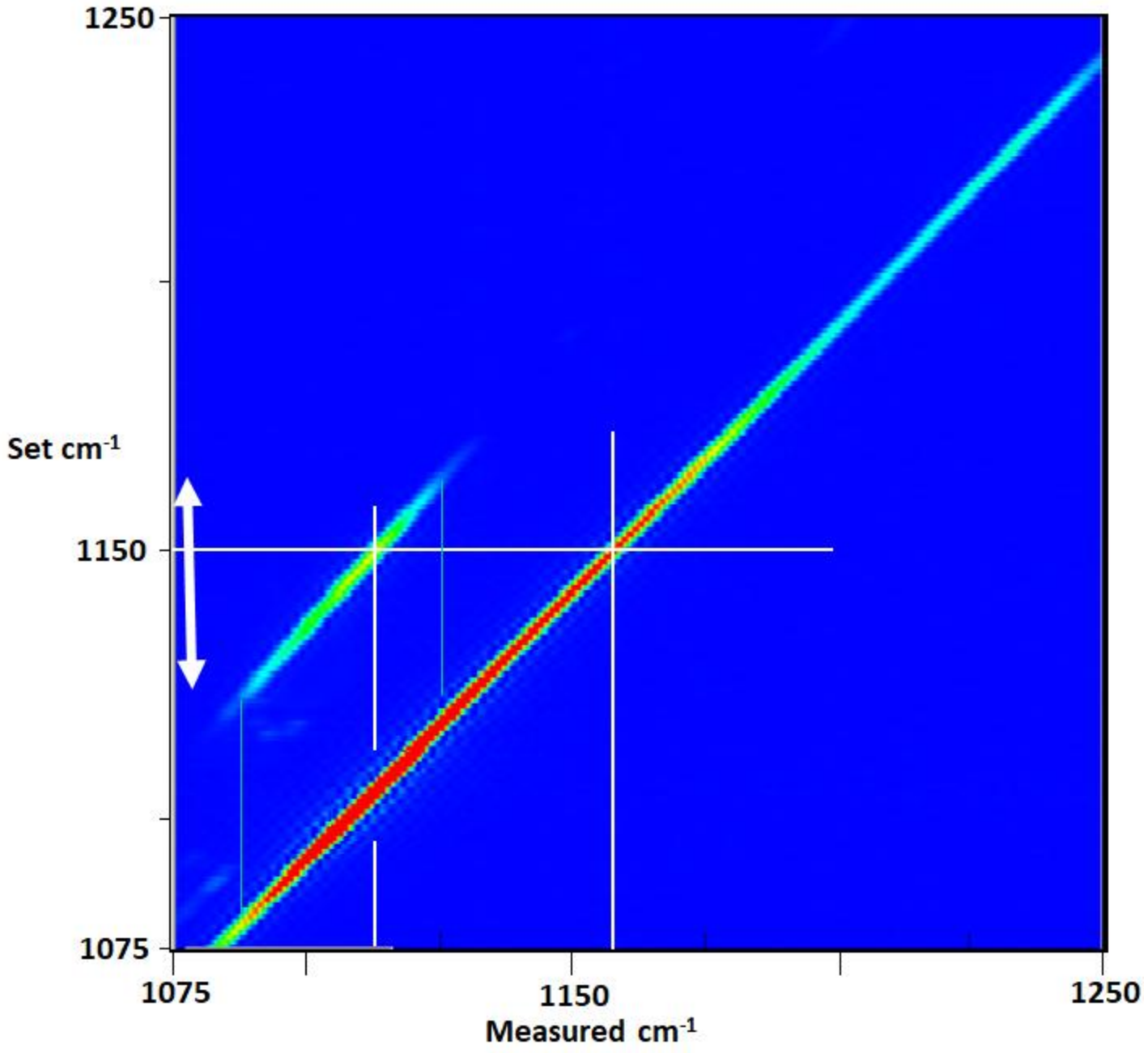


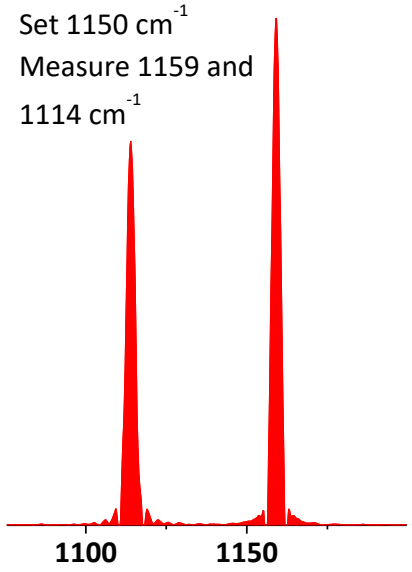


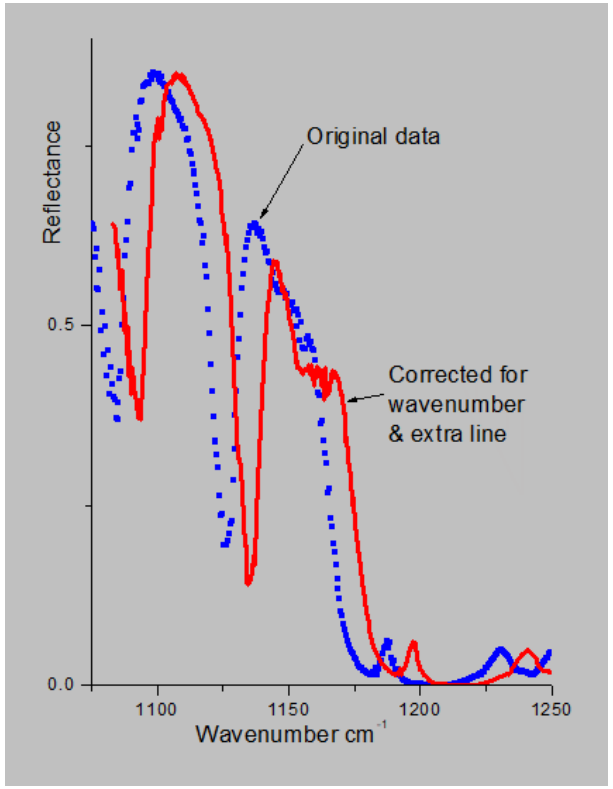
Laser Performance

- Source based spectroscopy
- Wavenumber linearity
- Uniqueness

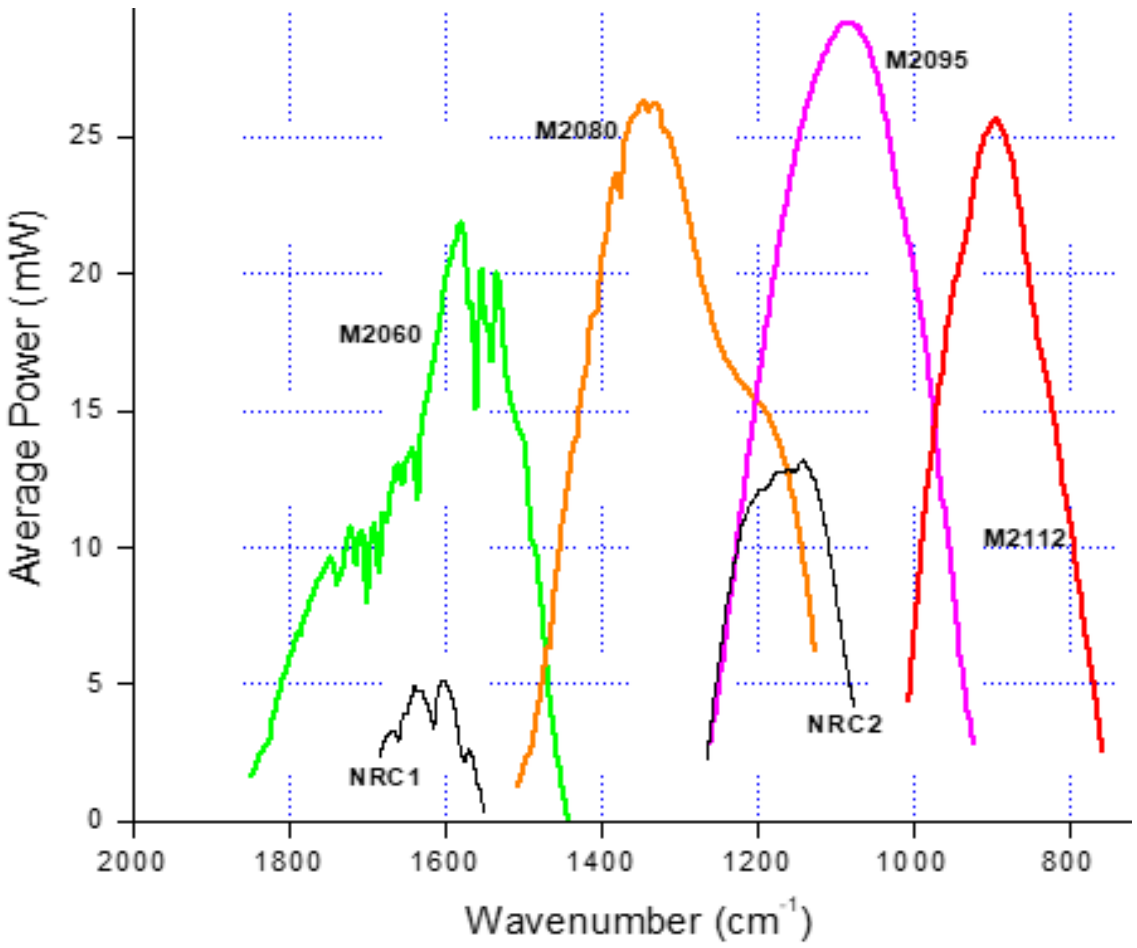
- Wavenumber offset
- For settings 1125 to 1160 cm^{-1}: two lines
- Correction algorithm
- Lower wavenumber (by 45 cm^{-1}) line thwarted

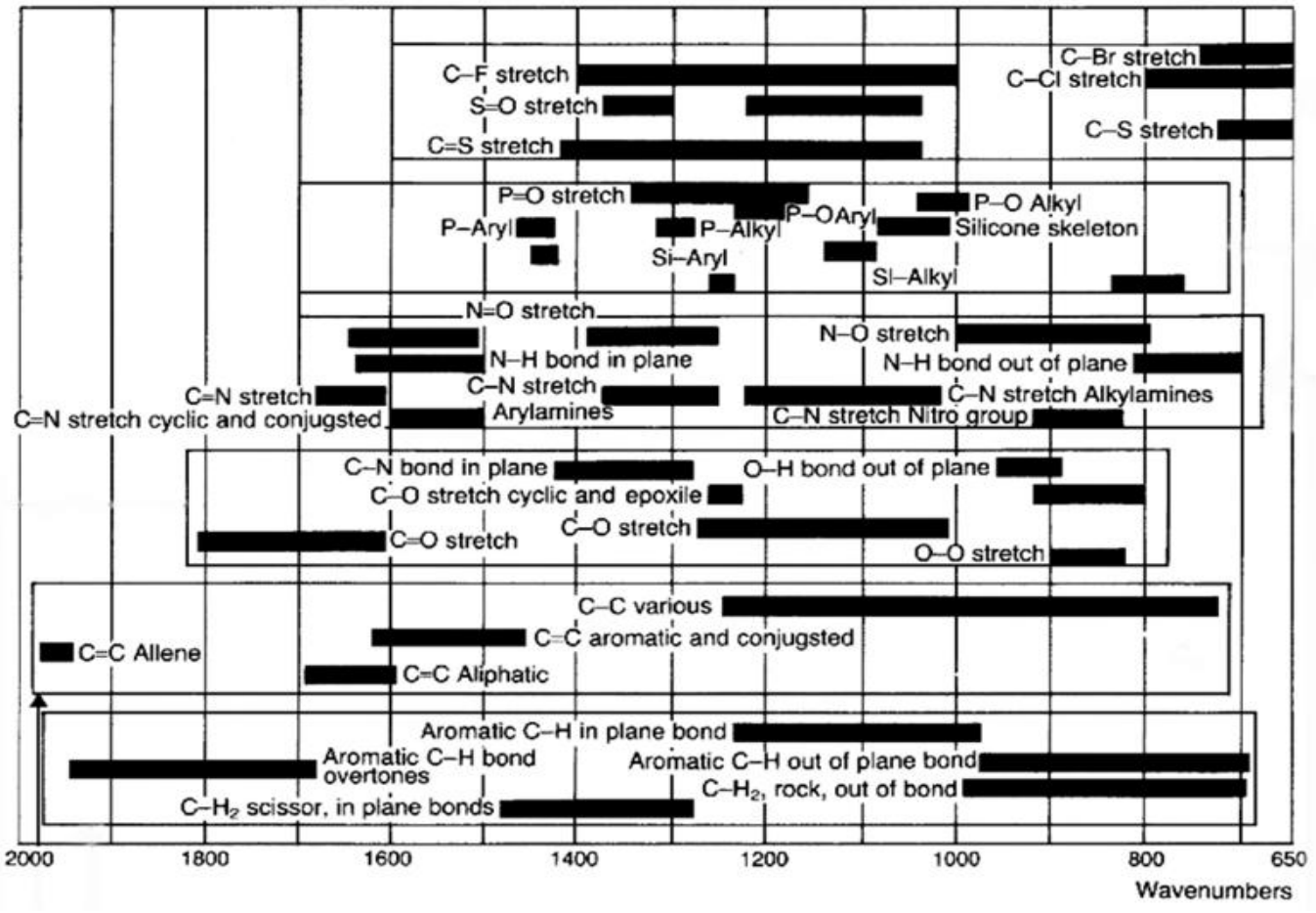






Performance Improvements DLS QCLs – Tuning Range and the Fingerprint Range





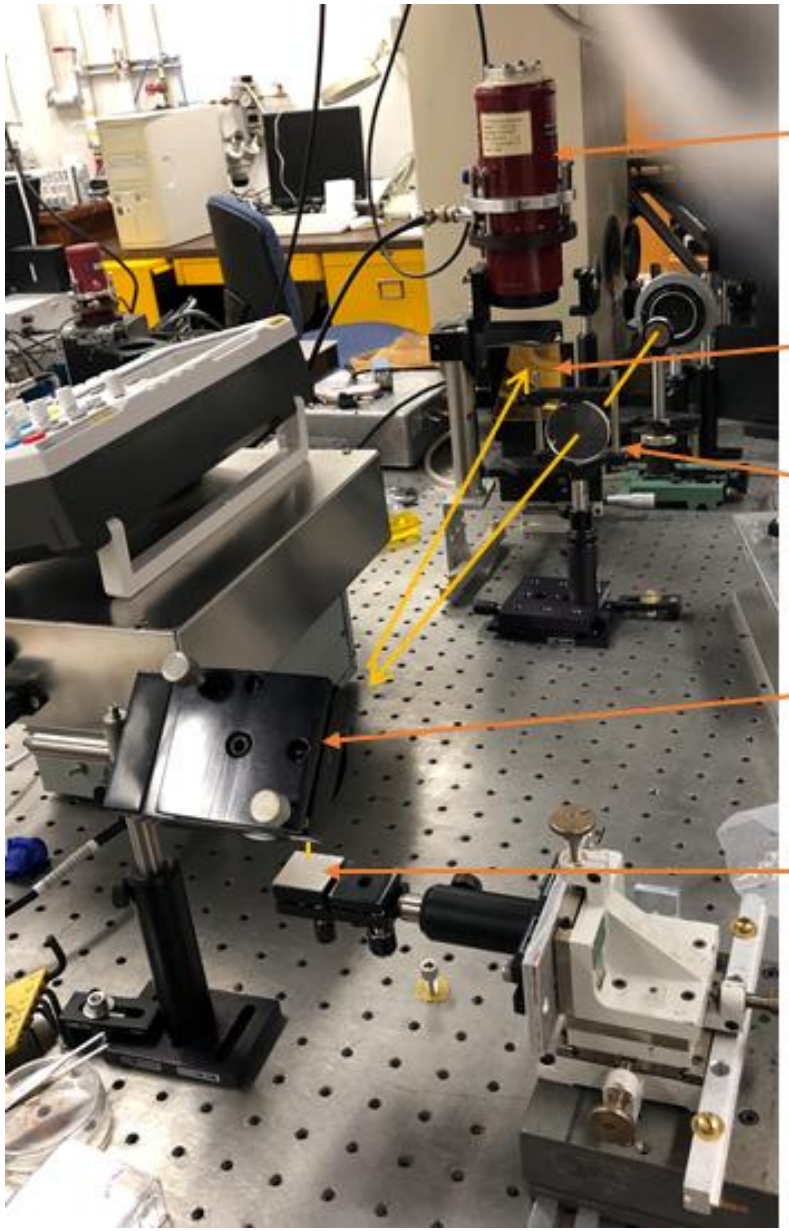
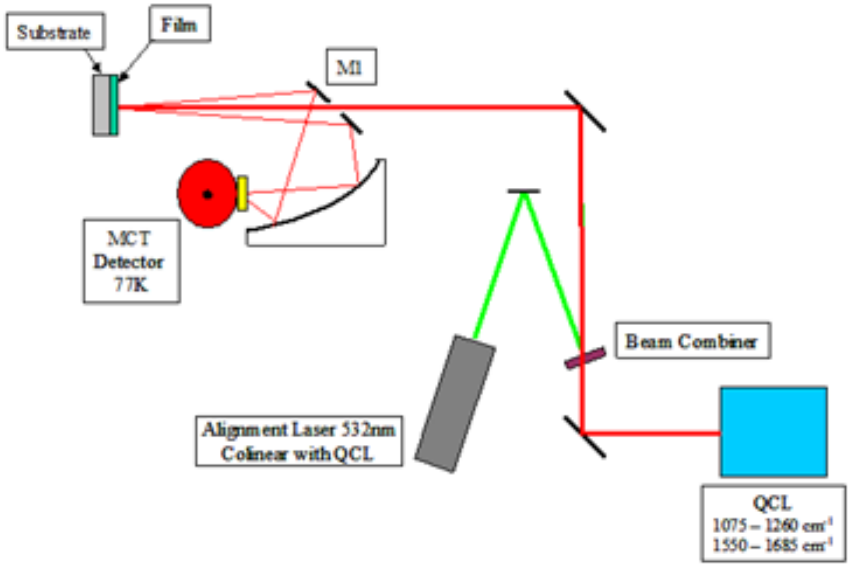
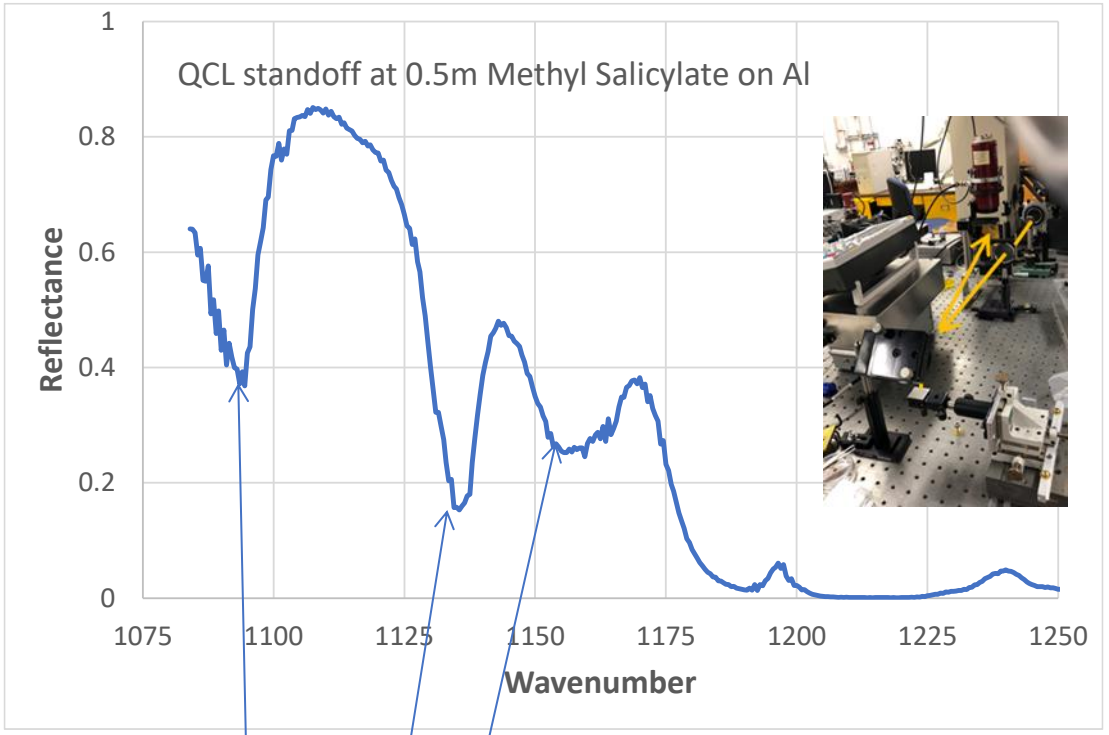


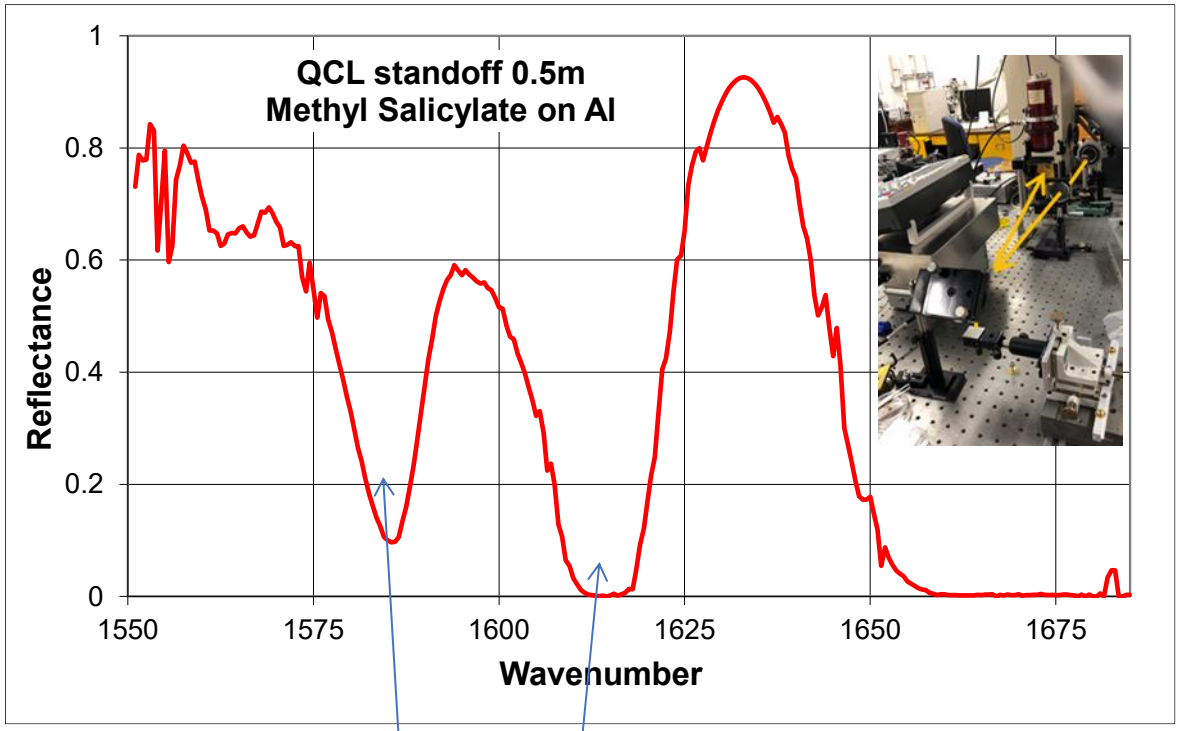
Table Top Standoff Detection System

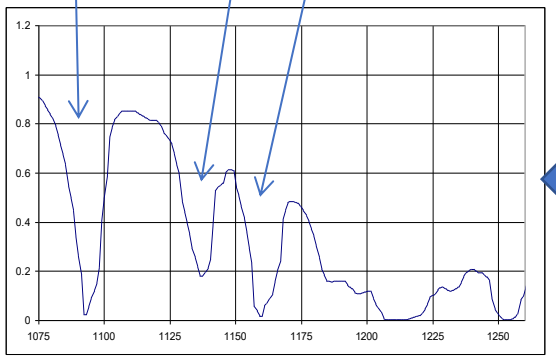
Distance – laser optics to sample 0.5 m
Distance – sample to collection optics 0.55 m
Reflectance angle – 4 degrees off normal
Quantum cascade lasers (QCLs) are the source
Spot size on sample ~ 2 mm diameter
QCL #1: 1075 to 1250 cm^{-1} (9.3 to 8 µm)
QCL #2: 1550 to 1685 cm^{-1} (6.45 to 5.93 µm)
Detector mercury cadmium telluride photoconductor (77K)
Spectra obtained by step scanning the lasers



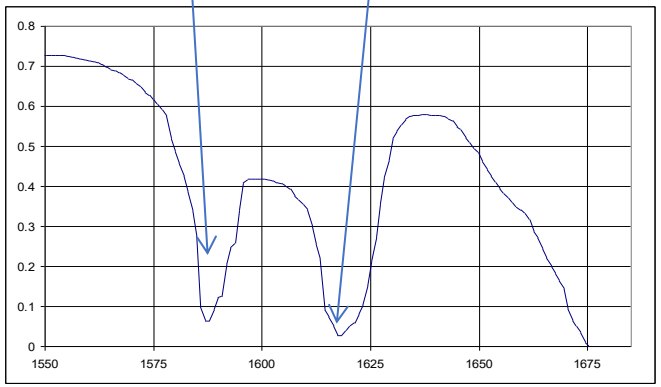
Methyl Salicylate Liquid on Aluminum: Standoff at 0.5 m ~14 µm





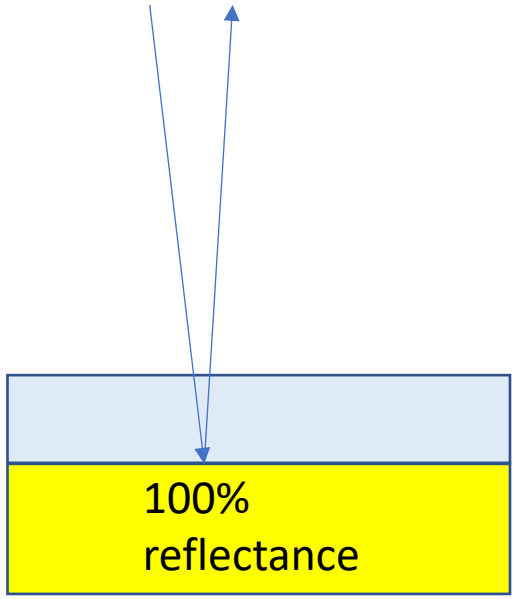


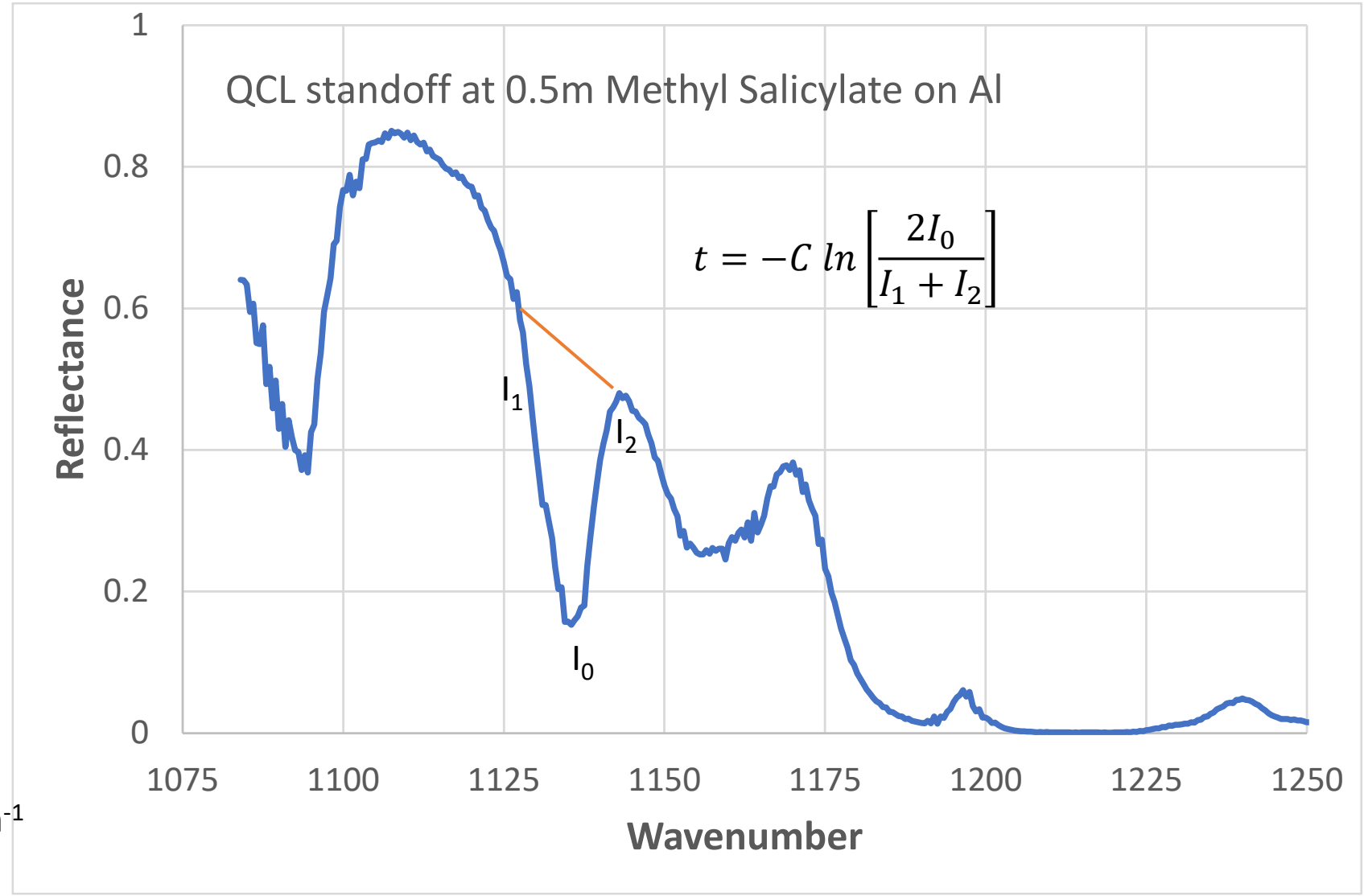
NIST Database Transmittance Spectra for 100 µm Methyl Salicylate



TAKEAWAY
Reasonable identification of the chemical.
S/N implies sensitivity to much thinner films possible.

Methyl Salicylate Thickness estimation





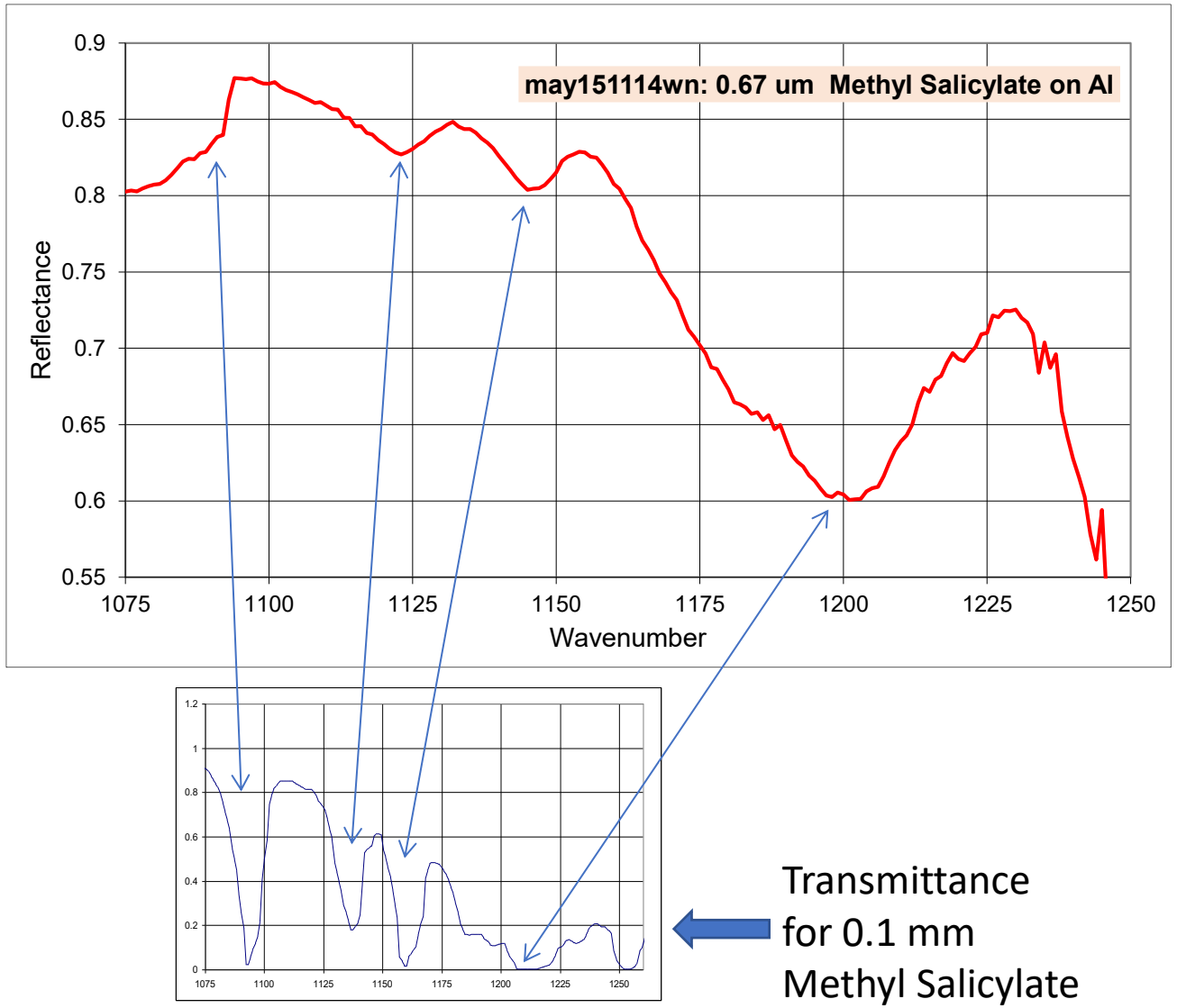
$t = -13.9\ ln\left[\frac{2I_0}{I_1+I_2}\right]$ at 1087 cm^{-1}

$t = -38.1\ ln\left[\frac{2I_0}{I_1+I_2}\right]$ at 1130 cm^{-1}

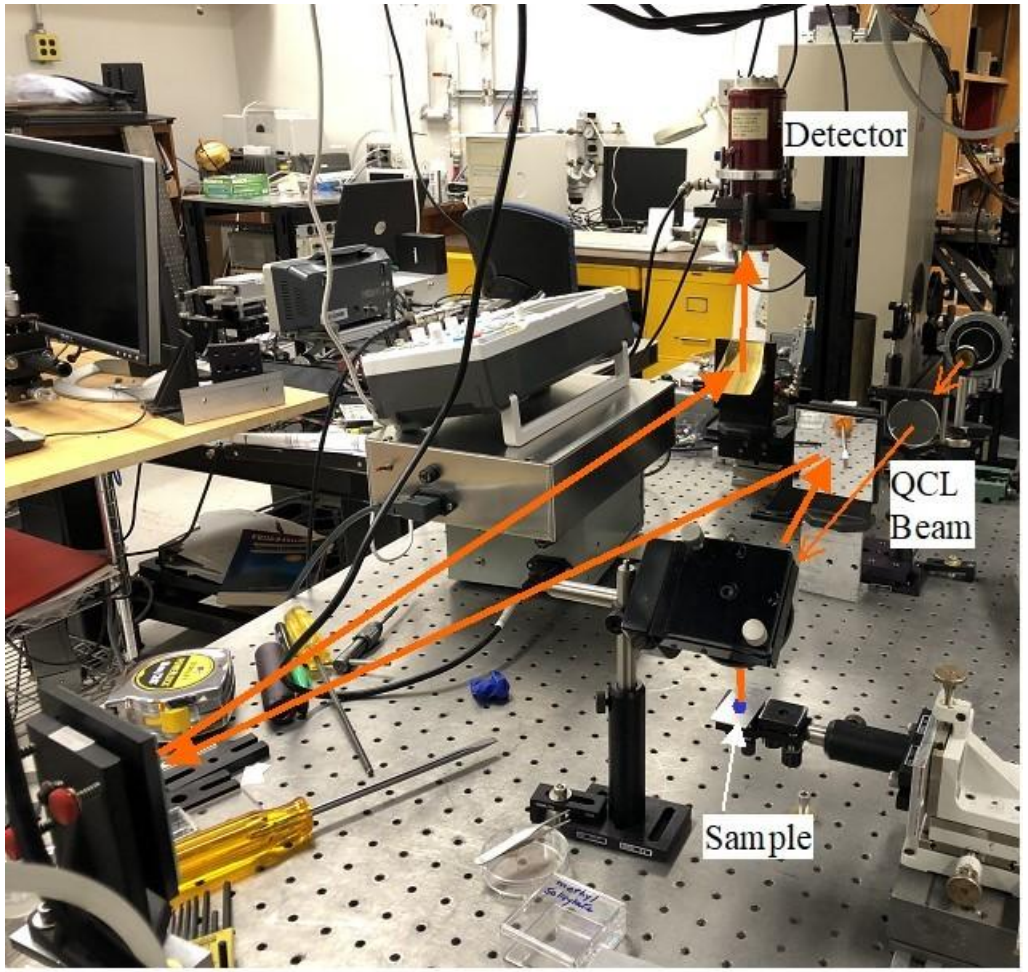
$t \approx 14 \pm 1\mu m$

$t \sim lnR$

Standoff at 1.8 m for 0.67 µm of Methyl Salicylate



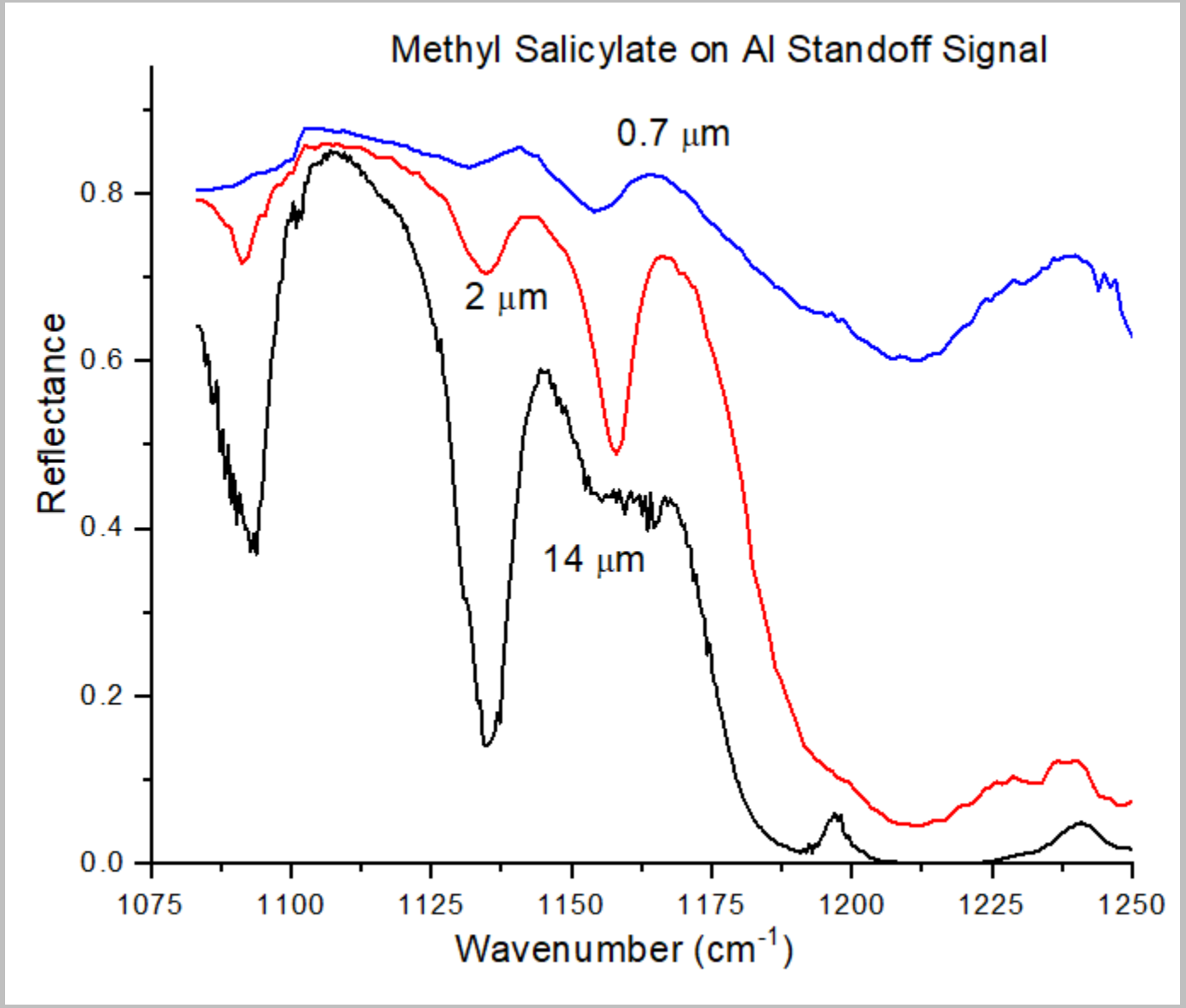
Transmittance for 0.1 mm Methyl Salicylate



Baseline improved with spatial filter.
S/N indicates thinner films possible.

Methyl Salicylate on Al: Data for R vs Film Thickness

- Three film thicknesses
- Reflectance declines with thickness
- But it this the case for all substrates?
- Useful to model the effect with thin film optics



High Reflectance Substrates: Reflectance Simulation for Methyl Salicylate Layers

About Substrate Constants

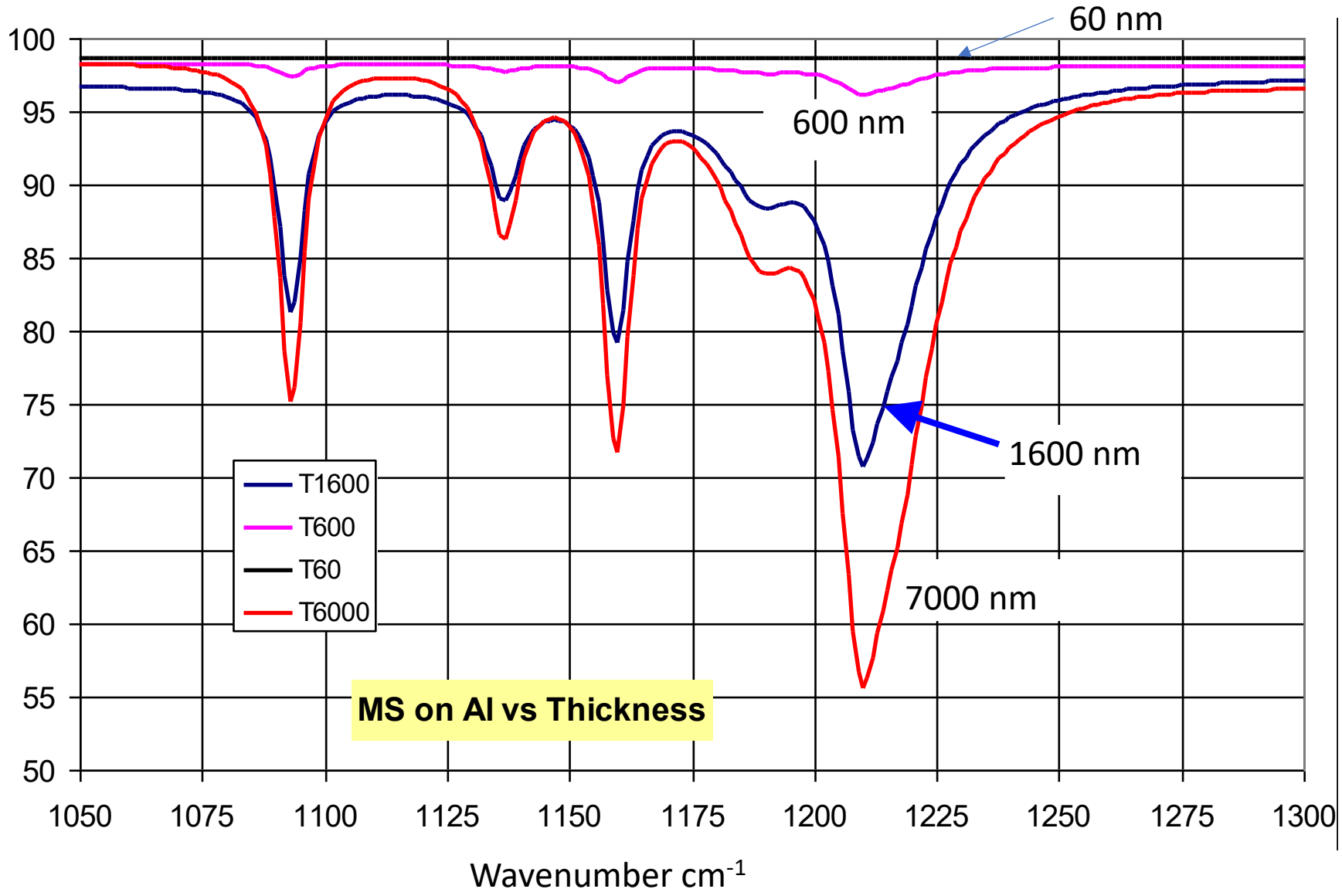
$$R = \frac{(n-1)^2+k^2}{(n+1)^2+k^2}$$

$$n_{sub} = 8.67$$

$$k_{sub} = 48.6$$

$$R_{sub} = 98.6\%$$

- Calculations done with IGOR using Hansen's formulation
- Reflectance DECREASES from the substrate value
- Now like double pass transmittance
- Absorption depths monotonic with thickness
- Interference noticeable but not large



Low Reflectance Substrates: Reflectance Simulation for Methyl Salicylate Layers

About Substrate Constants

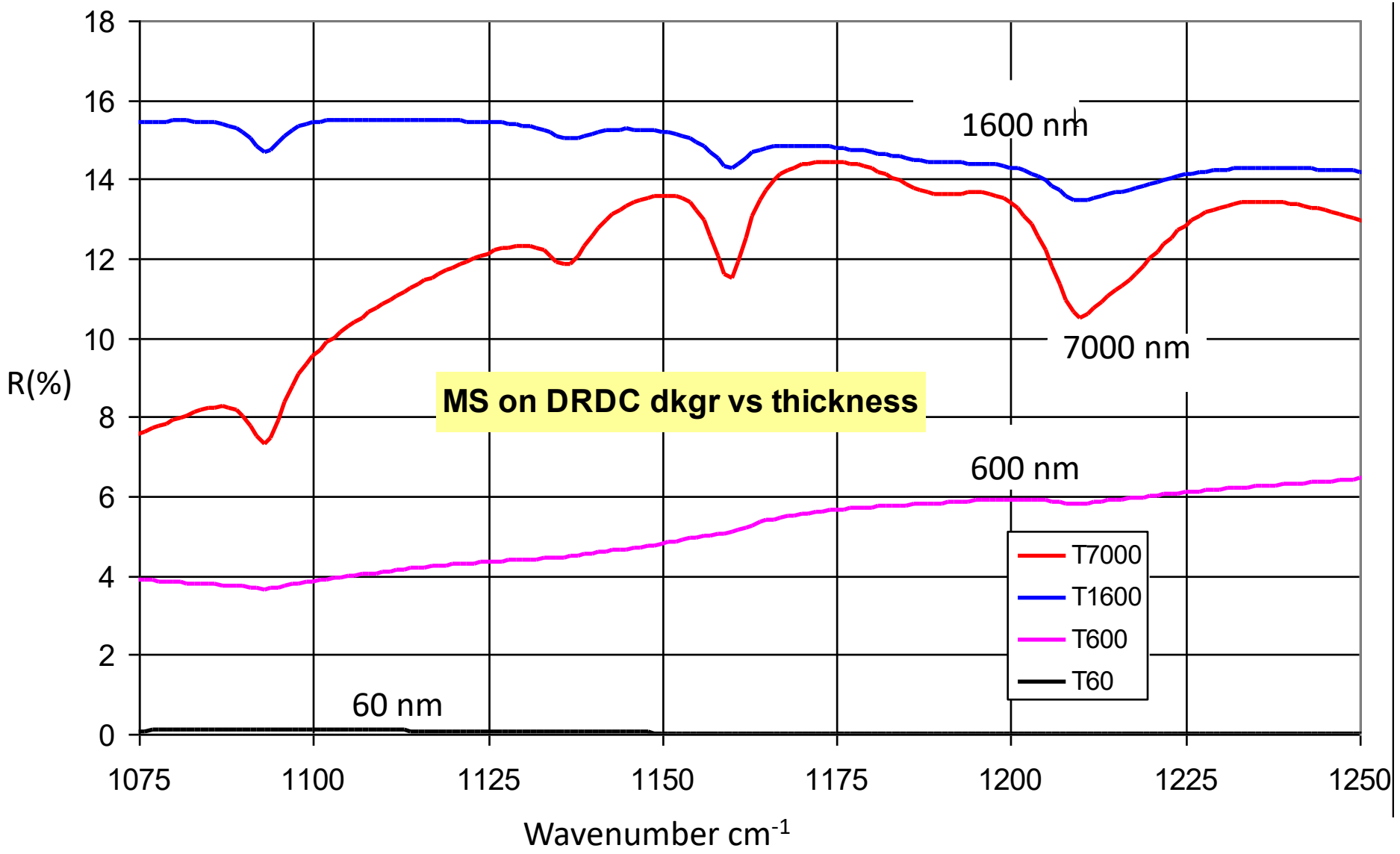
$$R = \frac{(n-1)^2+k^2}{(n+1)^2+k^2}$$

$n_{sub} = 1$

$k_{sub} = 0.09$

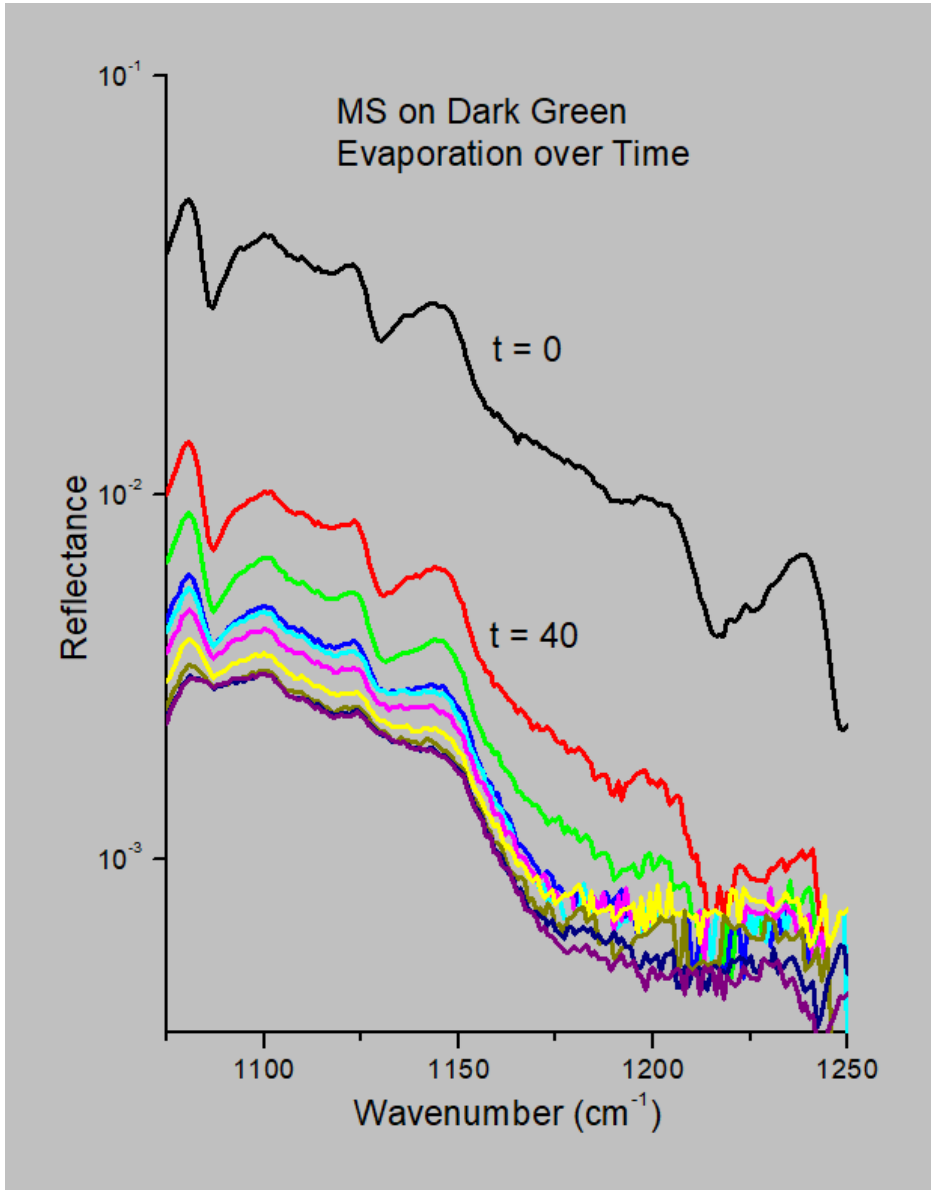
$R_{sub} = 0.2\%$

- Reflectance INCREASES from the substrate value
- Now like a free standing film
- Interference effects
- Absorption depths increase with thickness

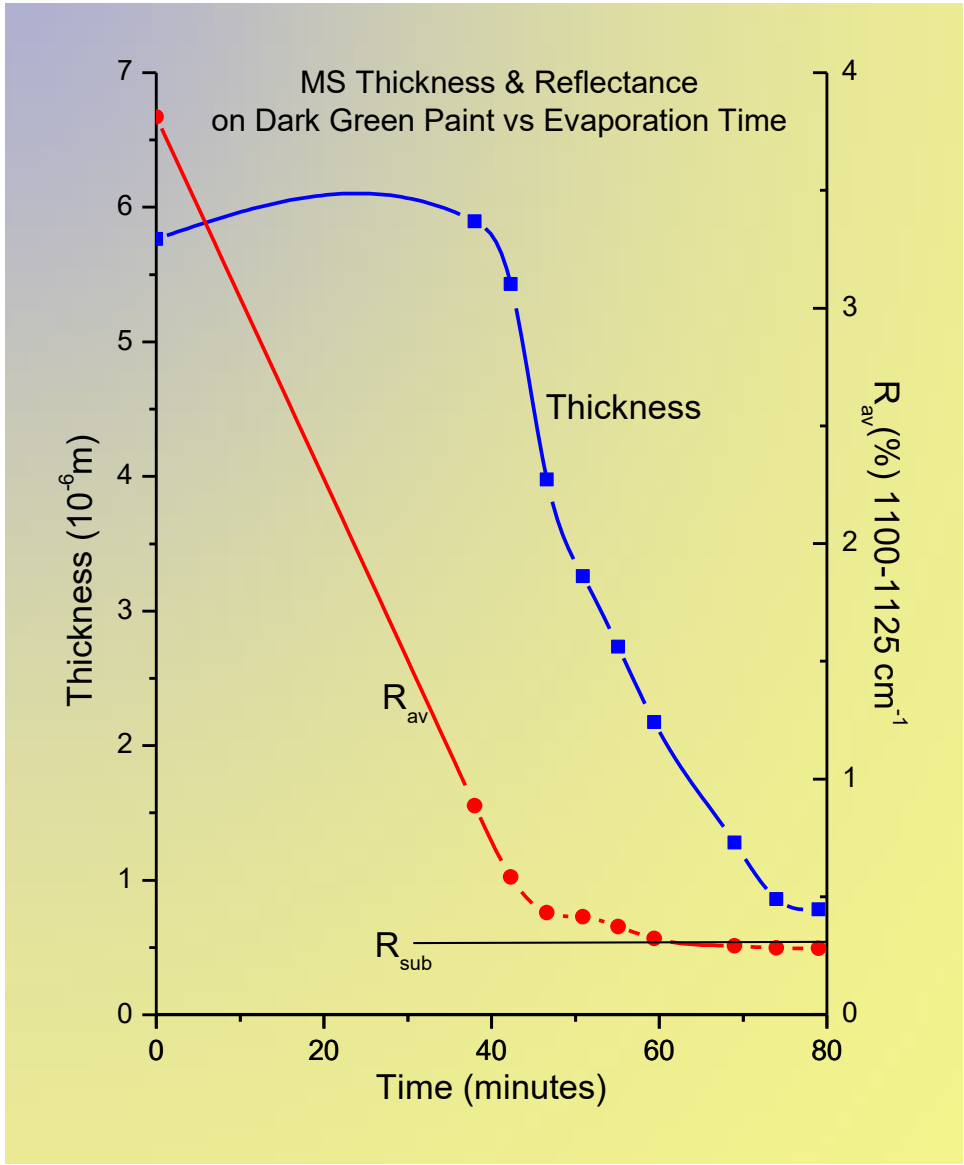


Low R Substrate: Methyl Salicylate Reflectance on Dark Green Paint on Metal

Thickness changes are clear clear on the log scale

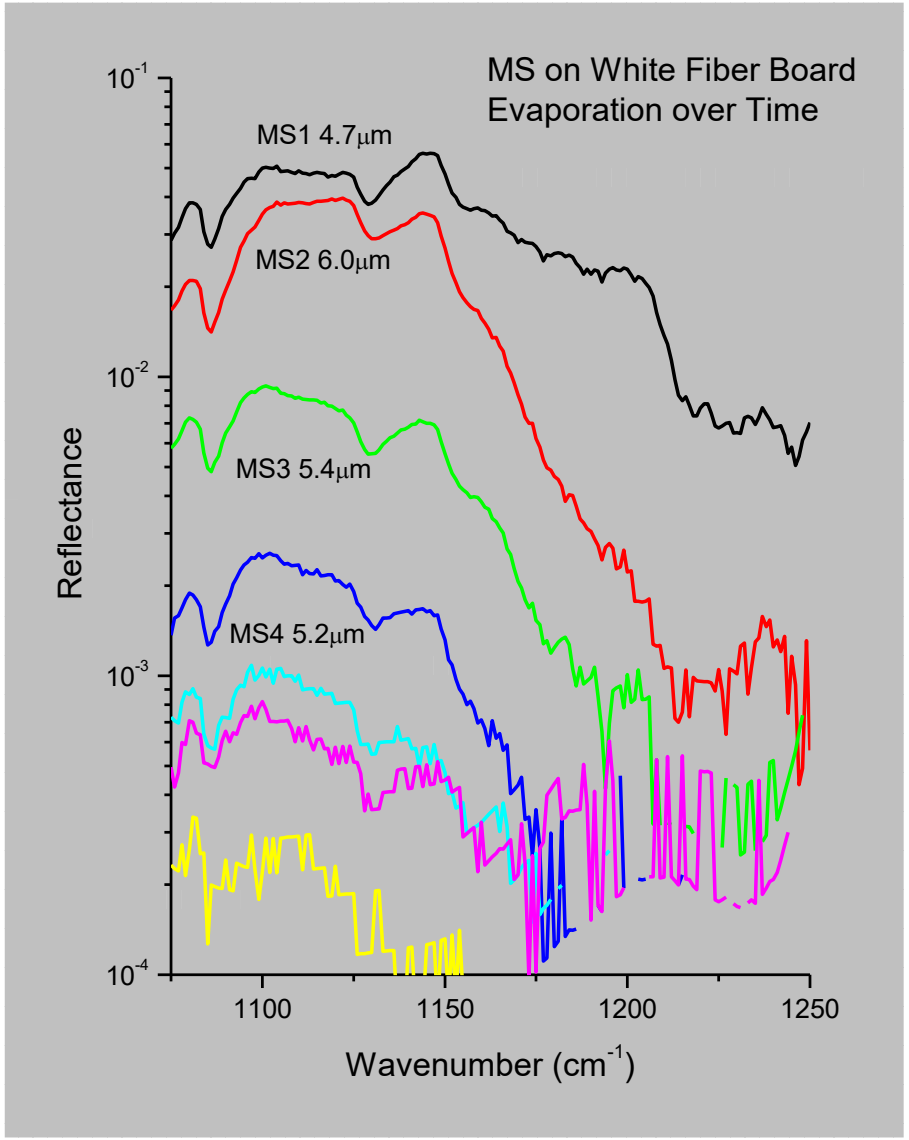


Thickness & coverage decline with time

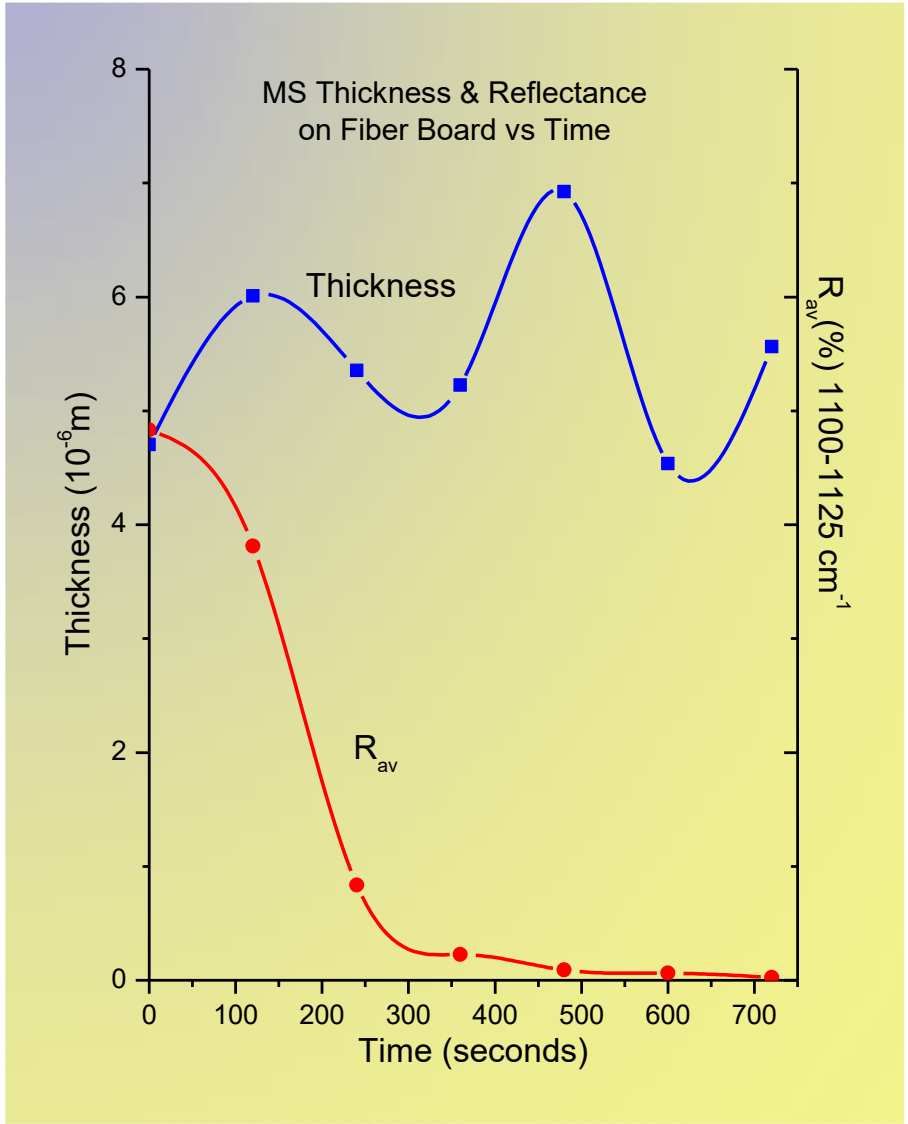


Porous Low R Substrate - Methyl Salicylate Reflectance on White Fiber Board

Constant thickness indicated by constant absorption depth on the log scale



Thickness unchanged with time Coverage declines rapidly



Summary

Standoff Detection of a Chemical Residue Using Quantum Cascade Lasers

Conclusions

Laser calibration important – spectral & spatial

Standoff distances in the couple of meter range

Sub micron layer thickness

Experiment and calculation, substrate properties

Outlook

New lasers – thinner residues, full spectrum ID

Larger distances both to laser and detector

Hyperspectral imaging with FPAs for chemical standoff images 800 to 1800 cm^{-1}