



# Towards a compact instrument to measure the volatile metabolites with submillimeter spectroscopy

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# Submillimeter spectroscopy of the volatile metabolome

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## Scientific case

### Microorganisms:

- own metabolism
- Volatile molecular output not unique?
- environmental growth factors?

B. A. Kimball, "Volatile metabolome: problems and prospects", Bioanalysis, 8(19) 2016

M. Sohrabi et al. "Volatile Organic Compounds as Novel Markers for the Detection of Bacterial Infections", Clin. Microbiol. Open Access, 3(3) 2014

A. Casaburi et al. "Bacterial populations and the volatilome associated to meat spoilage", Food Microbiol., 45, 2015

F. K. Tavares et al. "Amino Acid Catabolism and Generation of Volatiles by Lactic Acid Bacteria", J. Dairy Sci., 85(10) 2002

### Output variability, compatible with statistical classification analysis

M. Le Corvec et al. (DIAFIR, Rennes), "Mid-infrared fiber evanescent wave spectroscopy of serum allows fingerprinting of the hepatic metabolic status in mice," The Analyst, 2016

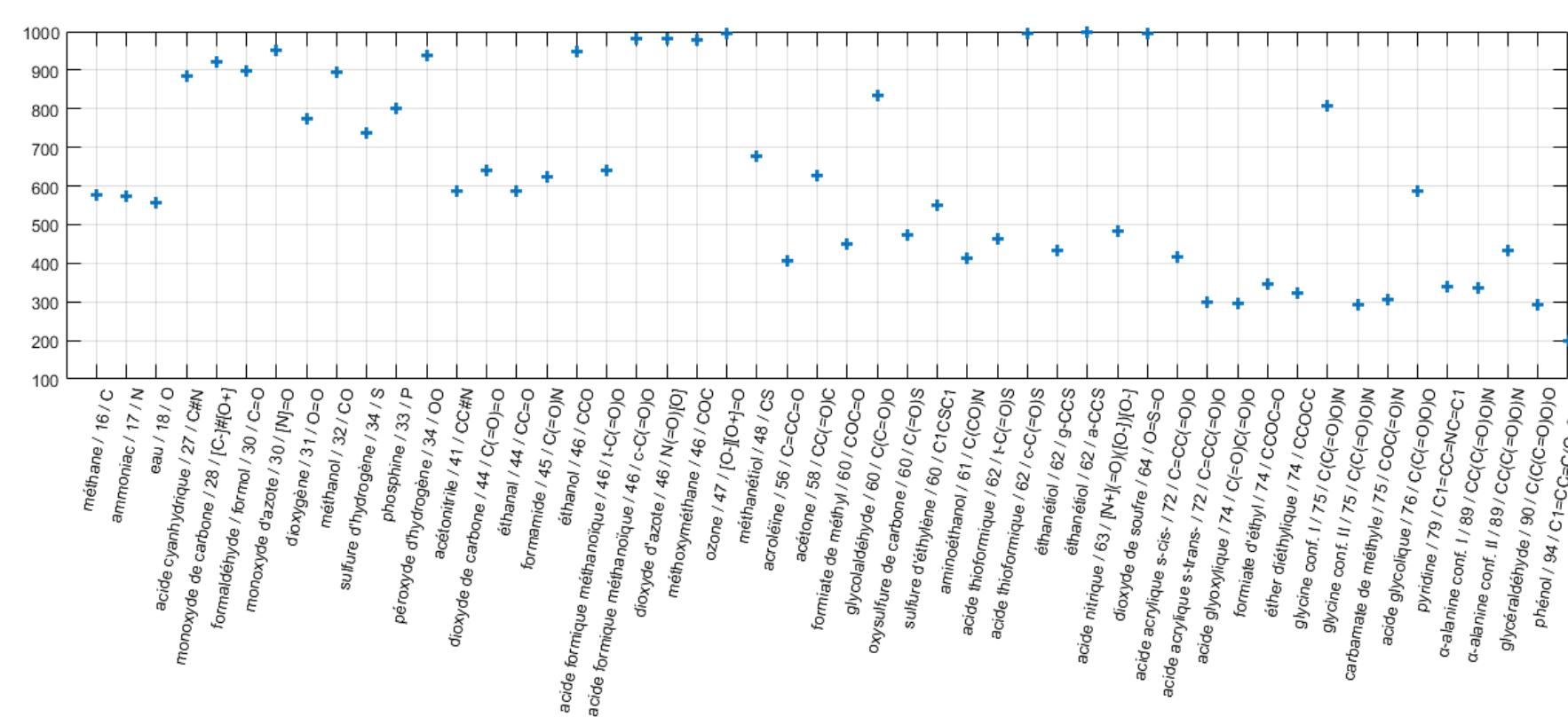
### Monitoring fermentation processes?

### Monitoring food spoilage?

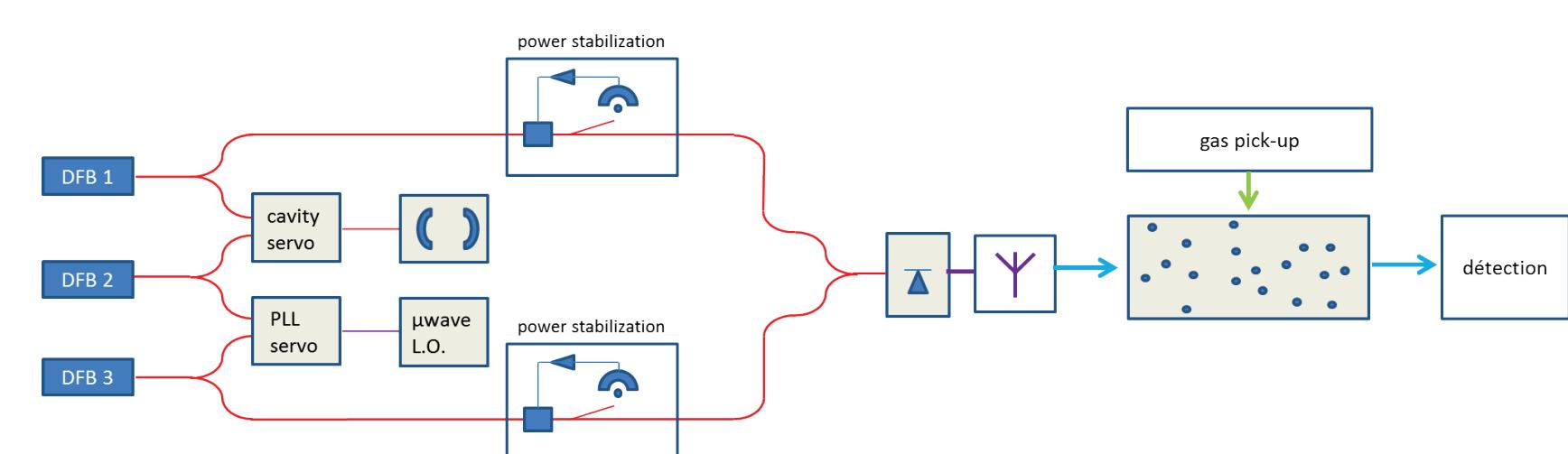
### Monitoring diseases?

## Instrument properties

- Large range of accessible frequencies  $\Leftrightarrow$  molecule diversity



- With optical telecommunication components



## Conclusion and outlook

- Robust synthesis of submm wave
  - in DC-580 GHz range
  - with photonics components
  - Step 1 GHz
  - Linewidth below requirements
- Construct continuously tunable synthesizer
- Build homodyne detection system
- Test on molecules in databases
- Test on real case

## Submillimeter spectroscopy

- Rotation-vibration resonances of whole molecules
- Resonances specific of molecular species
- Resonances (width  $\sim 100$  kHz) clearly distinct, contrary to IR spectroscopy

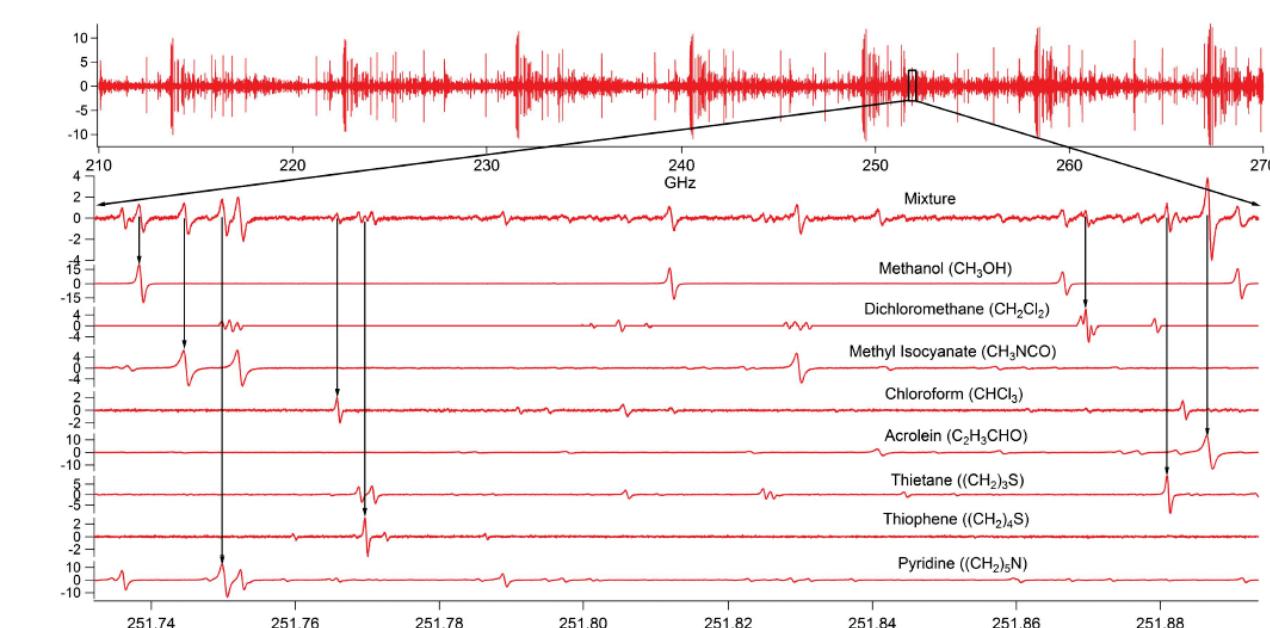
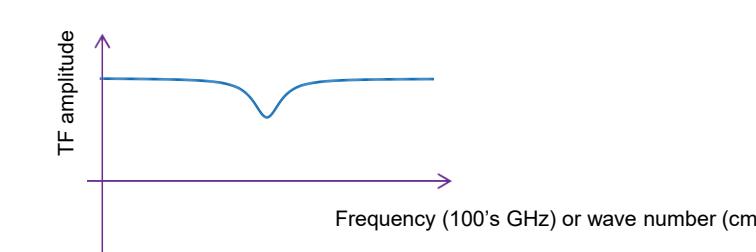
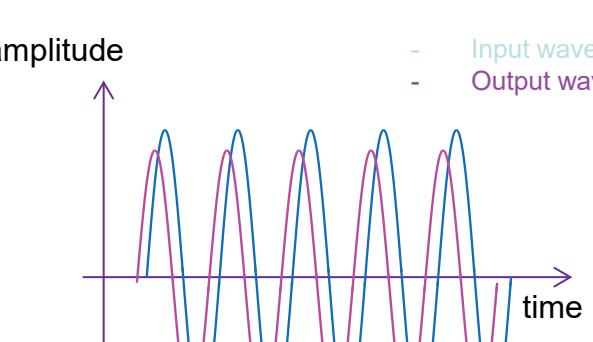
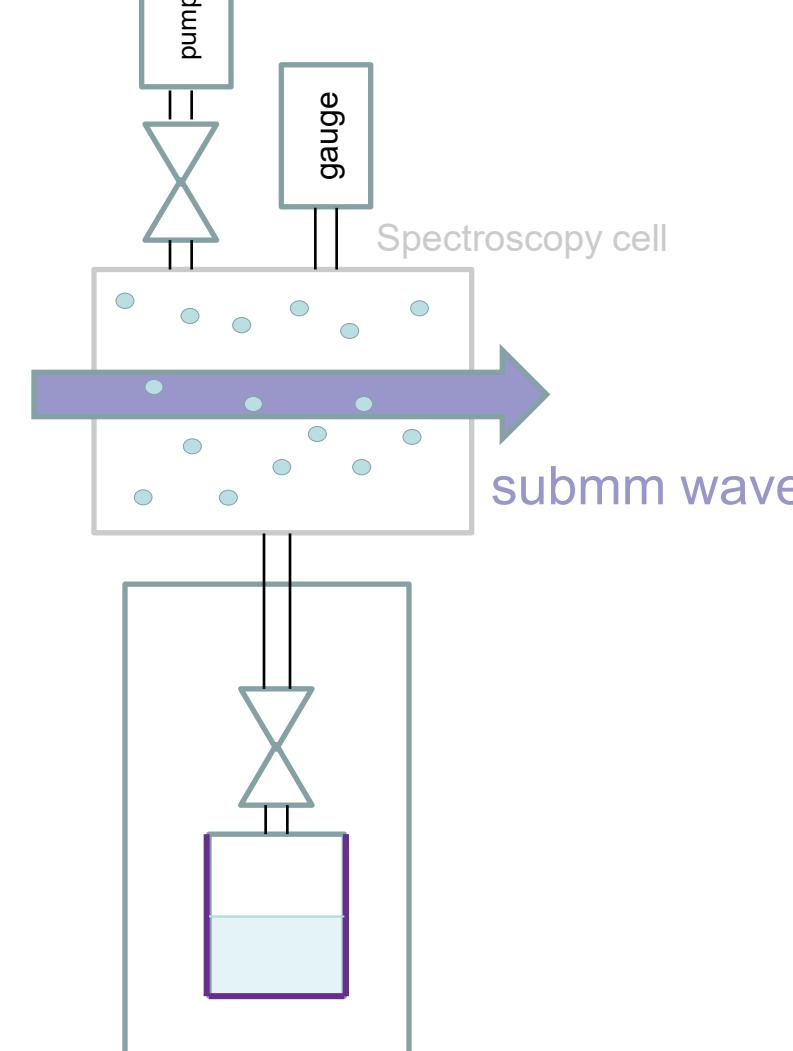


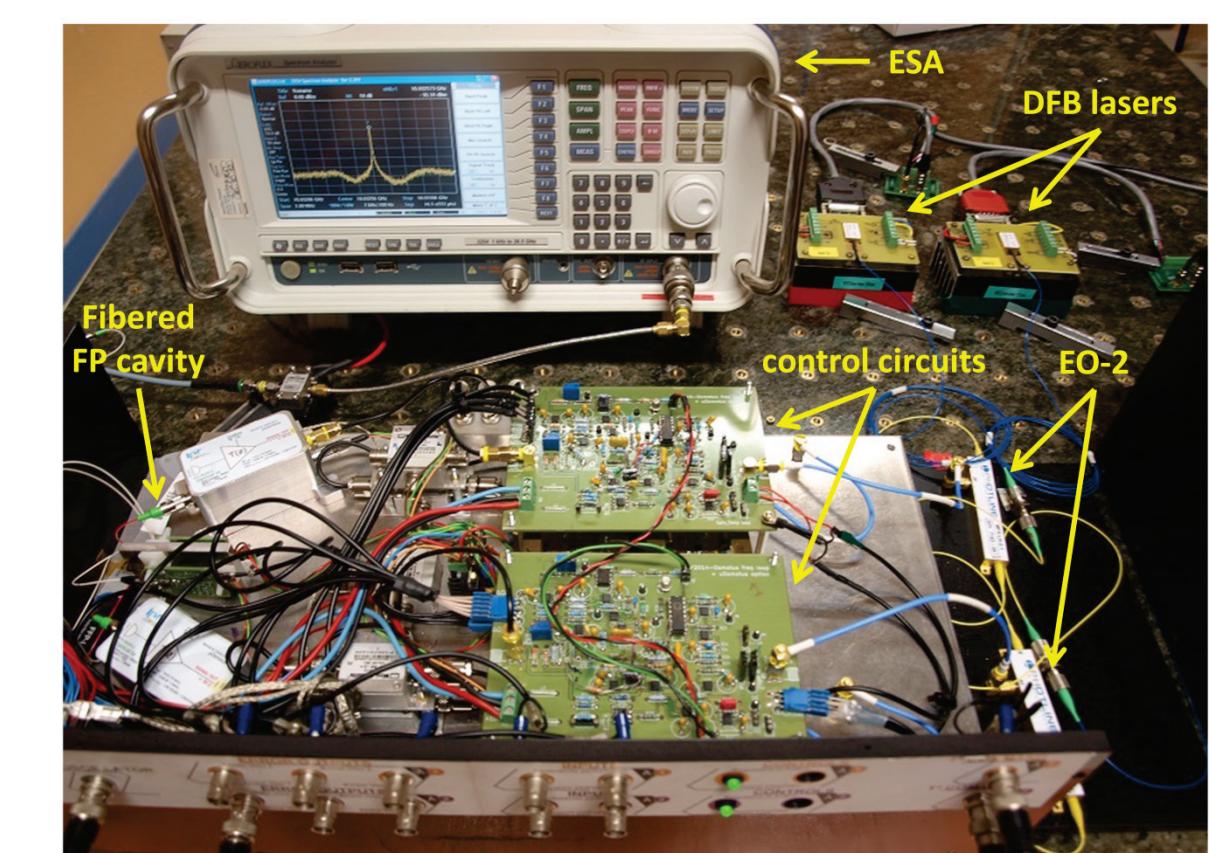
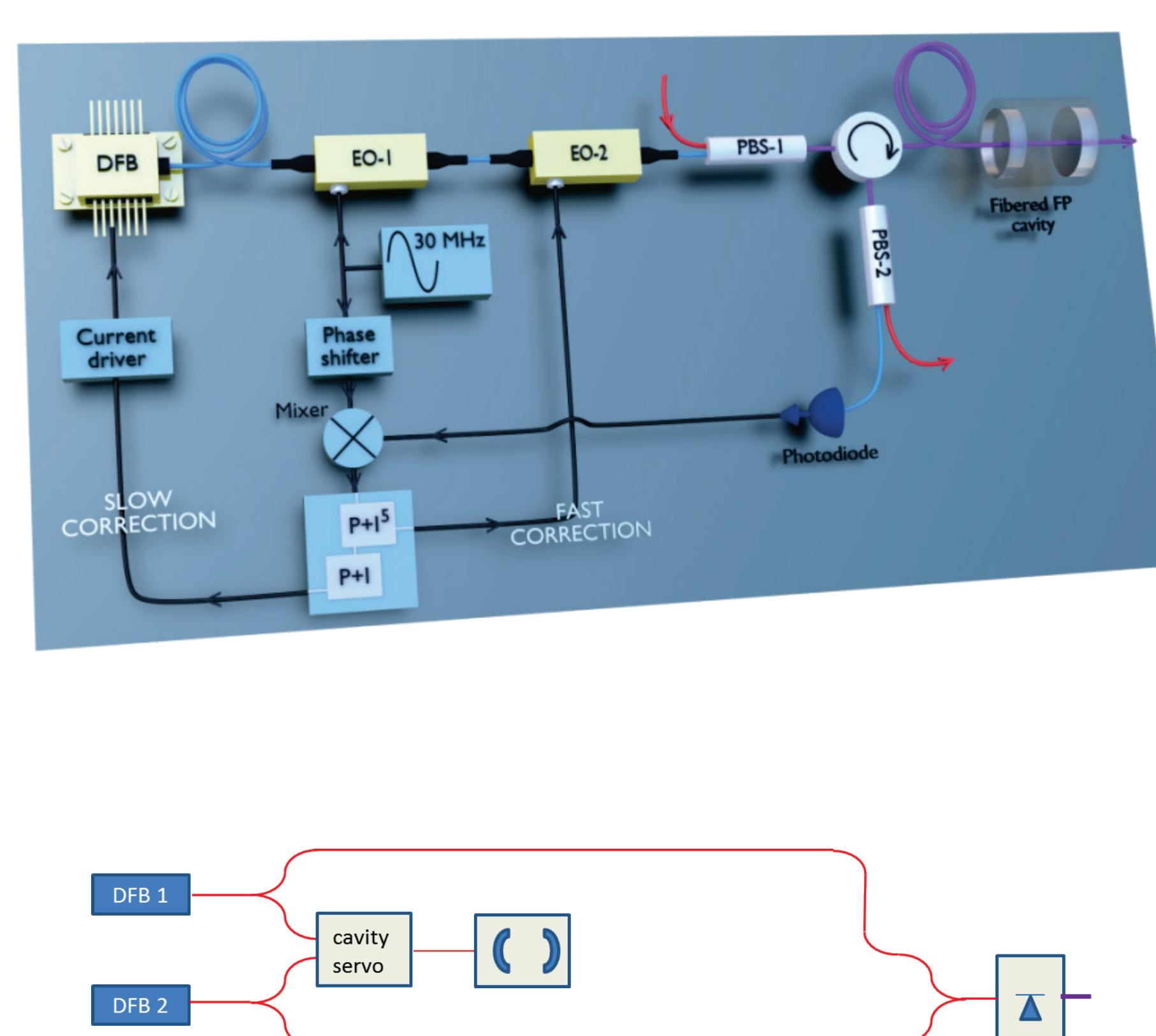
Fig. 1. Spectrum of a mixture of 14 gases in the region 210-270 GHz on a compressed scale (upper panel). The spectrum of a 0.15-GHz segment of this mixture (second panel). The library spectra of eight of these gases (panels three through ten).

C.F. Neese et al., "compact submillimeter/terahertz gas Sensor with efficient gas collection, preconcentration, an ppt sensitivity", IEEE sensors journal, 12 (8) 2012

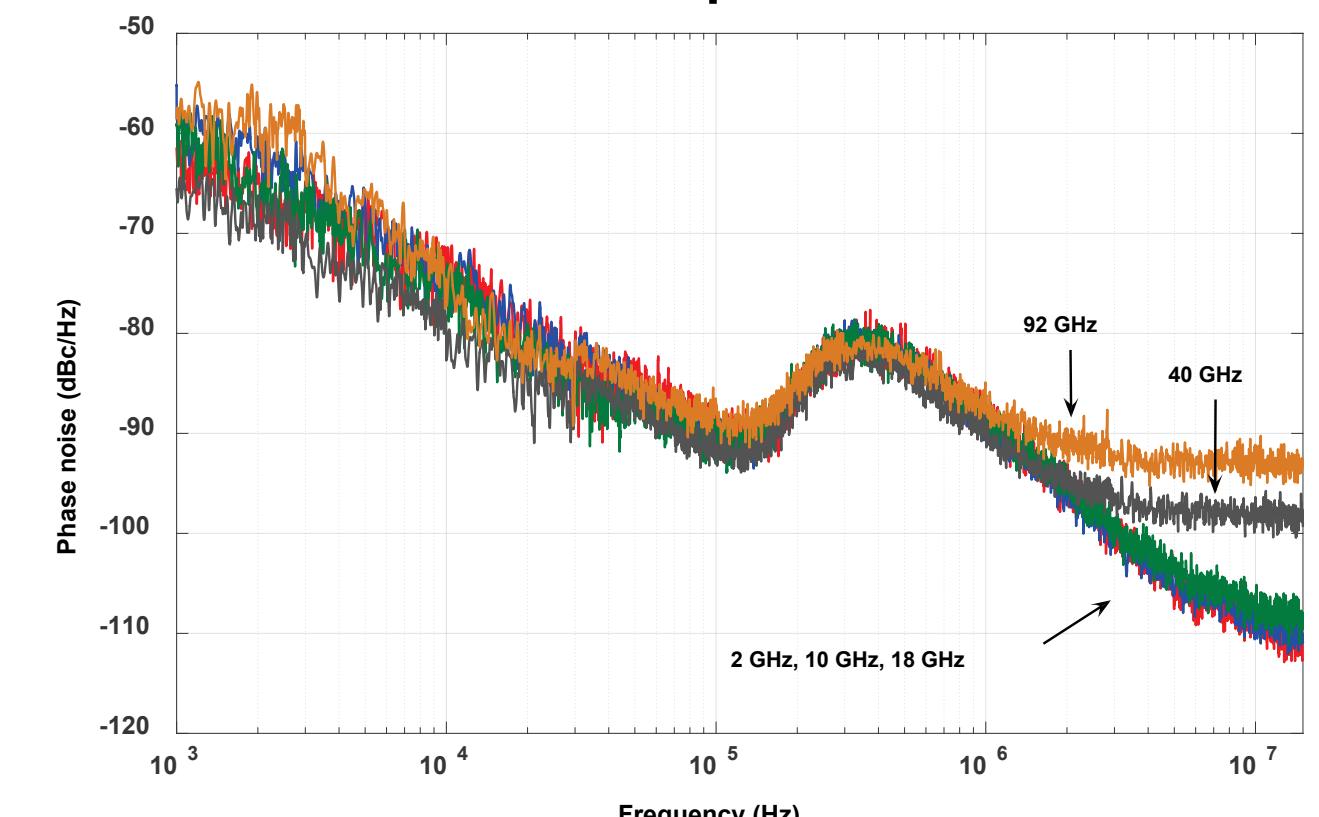
- No heating, no ionization: molecule integrity
- Prefers liquid phase sampling for solute molecules at room temperature and pressure
- Measurement at low pressure ( $< 1$  mbar)
- lots of molecules not in HITRAN/JPL/CDMS databases

## First results on wave synthesis

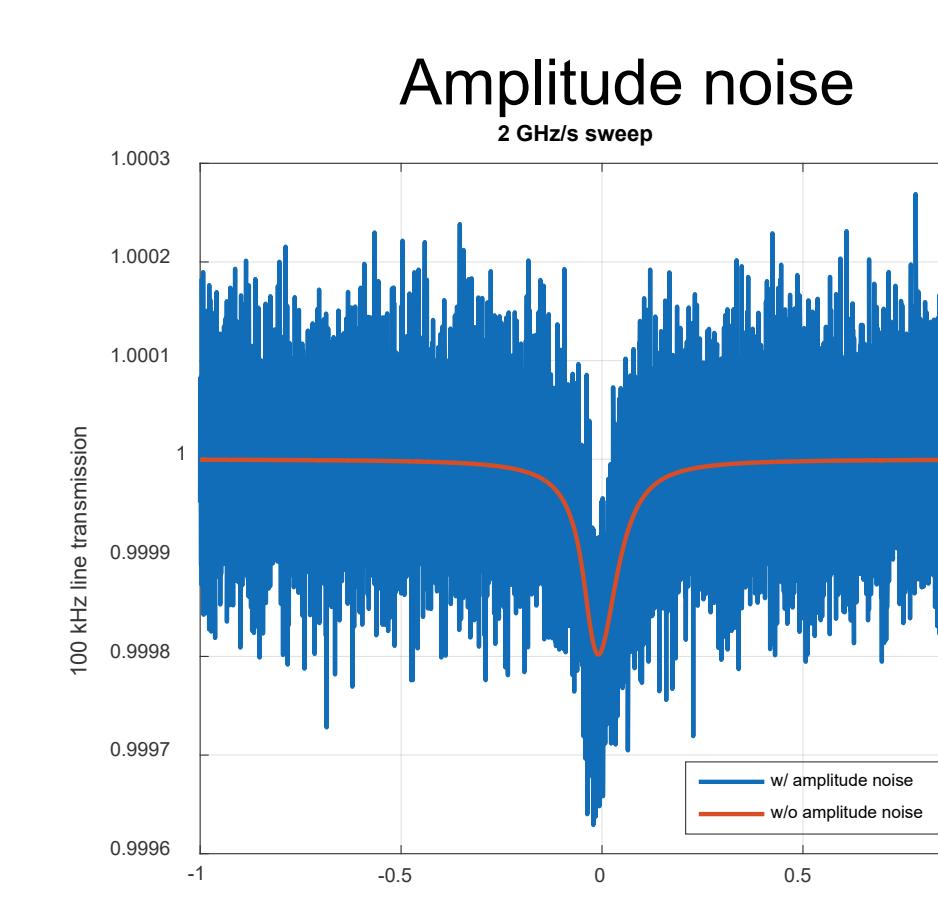
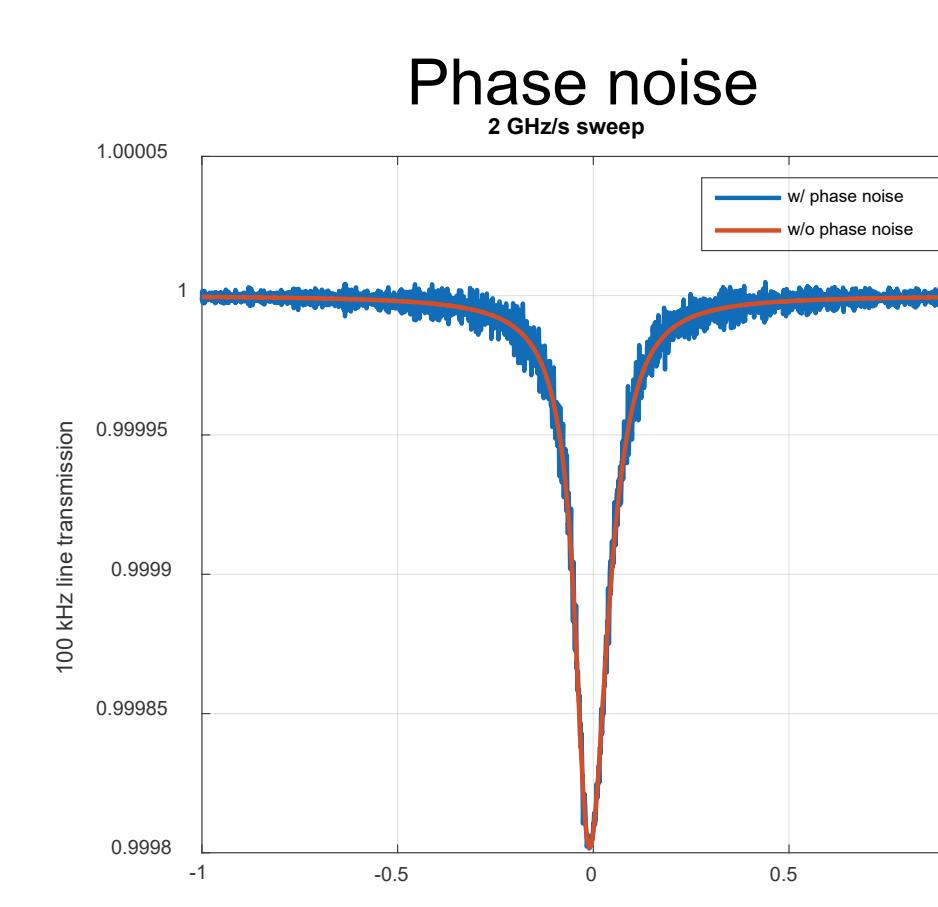
- One laser diode wavelength stabilization



### Measured phase noise



Modeling (non-linear) phase and amplitude noise effects in cell transmission:



Signal to noise depends on integration time, line strength, cell length...

**sub-ppm detectability seems achievable**