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

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

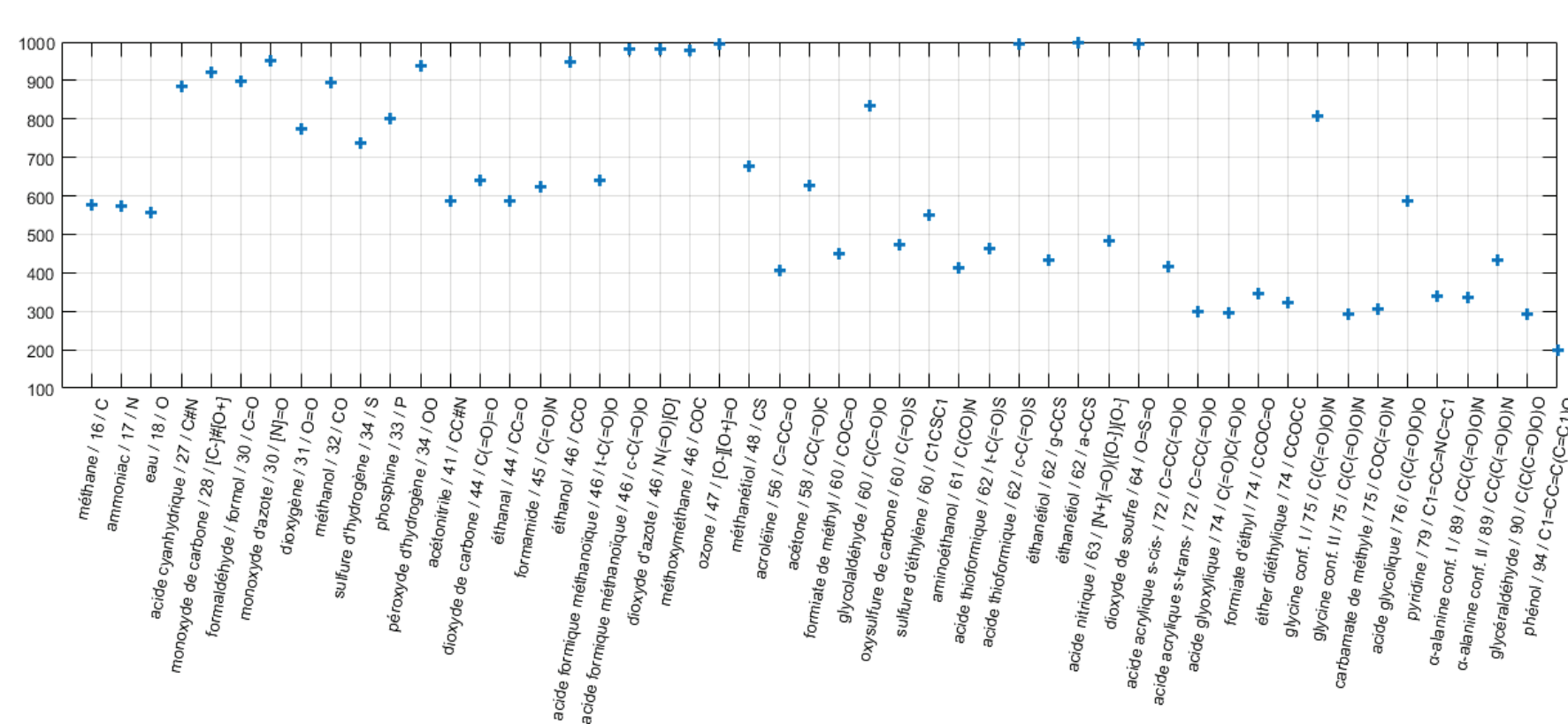
Output variability, compatible with statistical classification analysis

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

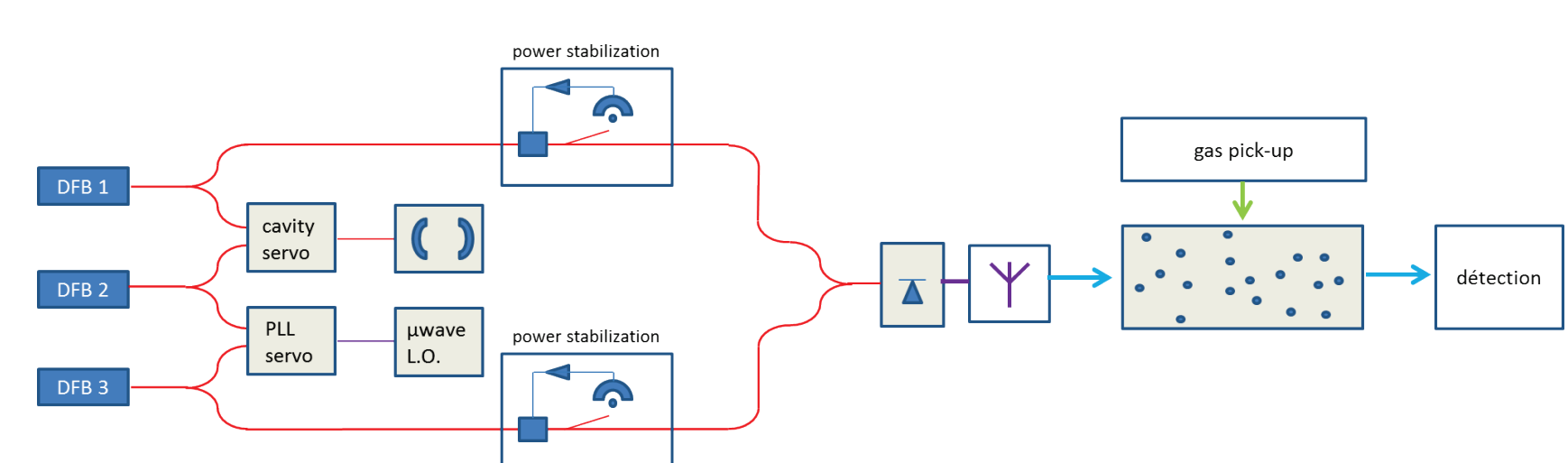
- Monitoring fermentation processes?**
- Monitoring food spoilage?**
- Monitoring diseases?**

Instrument properties

- Large range of accessible frequencies ↔ 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 ~100 kHz) clearly distinct, contrary to IR spectroscopy

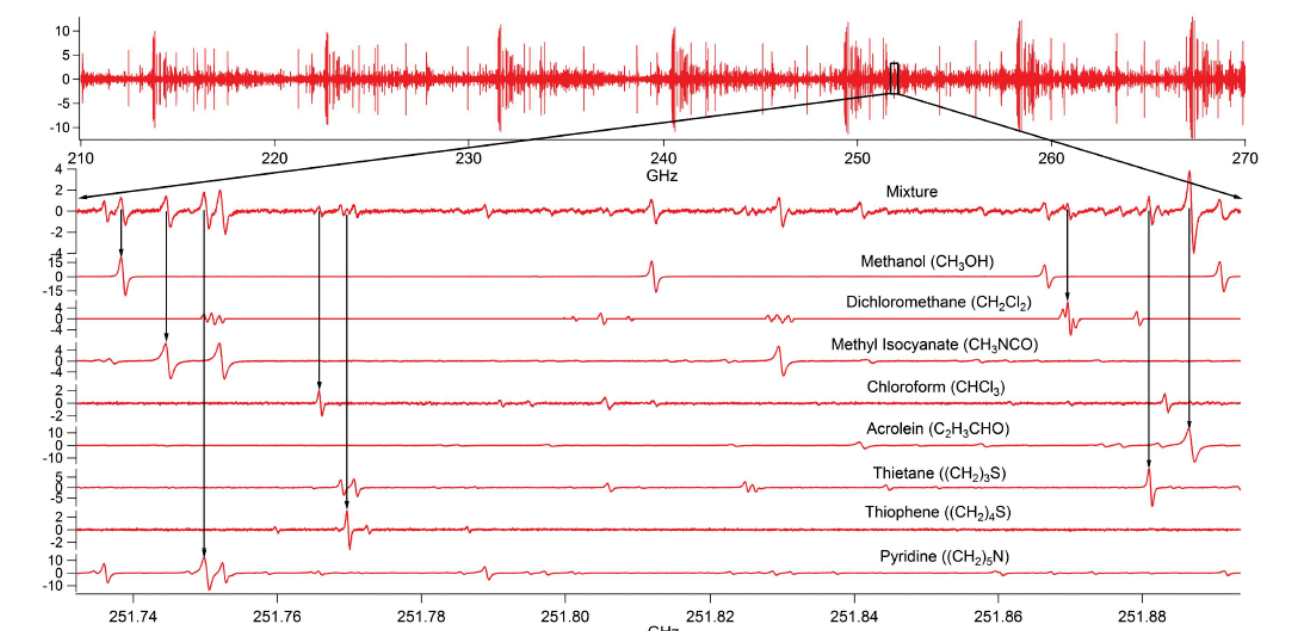
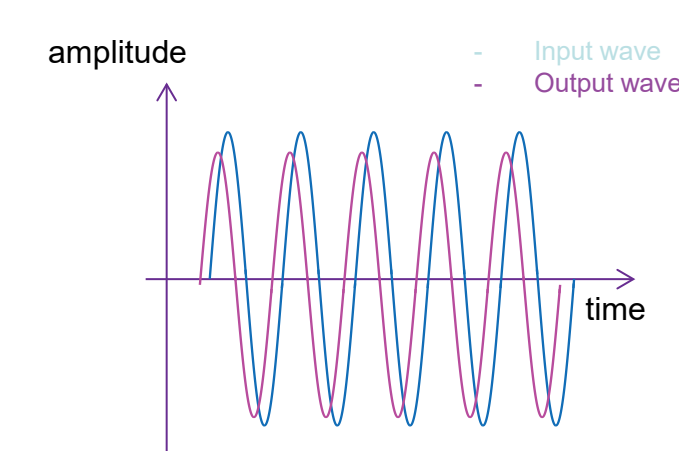
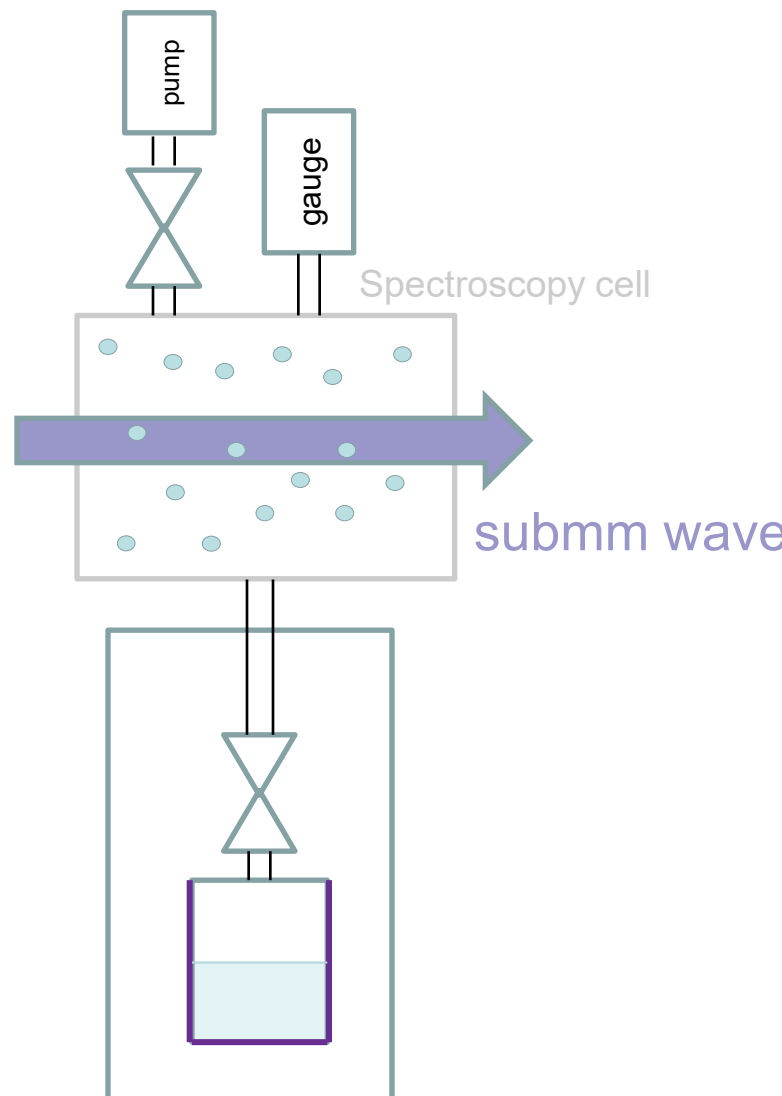


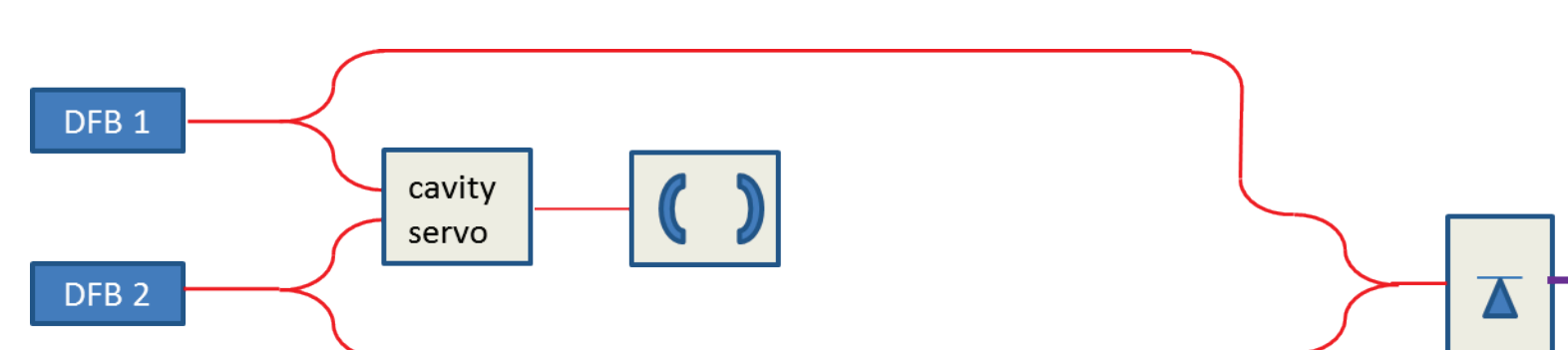
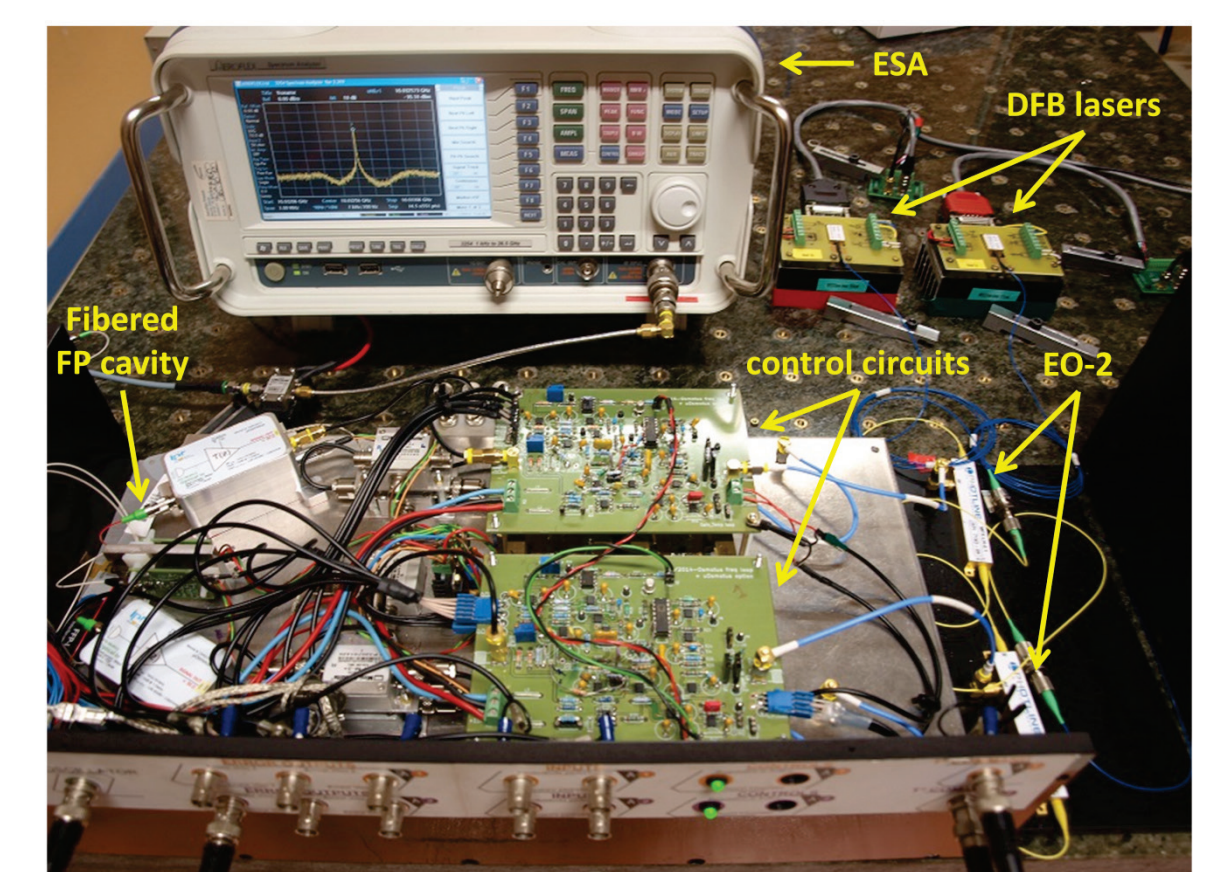
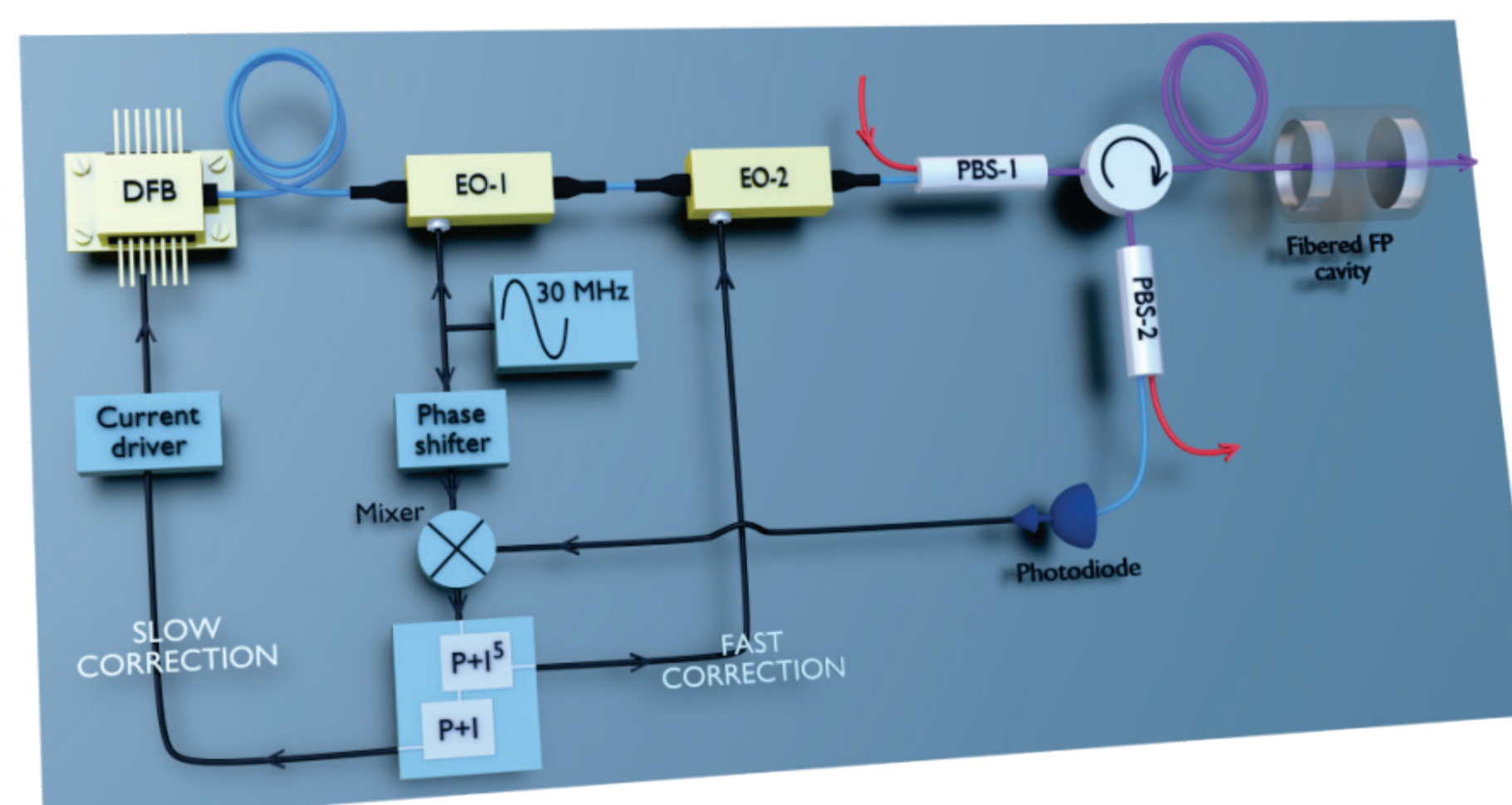
Fig. 1. Spectrum of a mixture of 14 gases in the region 210-270 GHz on a compressed scale (upper panel). The spectrum of a 0.15-GHz segment of this mixture (second panel). The library spectra of eight of these gases (panels three through ten).

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

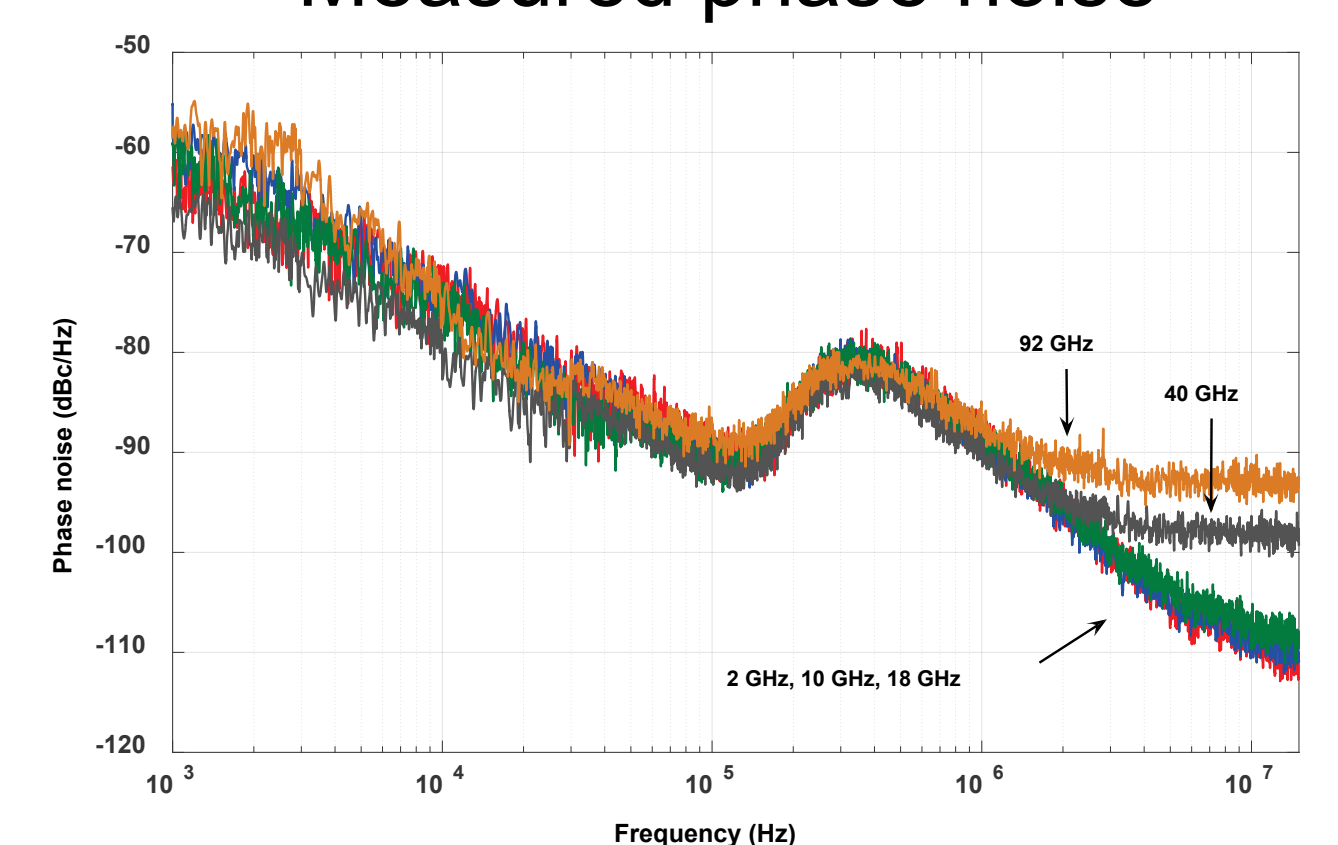
- No heating, no ionization: molecule integrity
- Prefers liquid phase sampling for solute molecules at room temperature and pressure
- Measurement at low pressure (< 1 mbar)
- lots of molecules not in HITRAN/JPL/CDMS databases

First results on wave synthesis

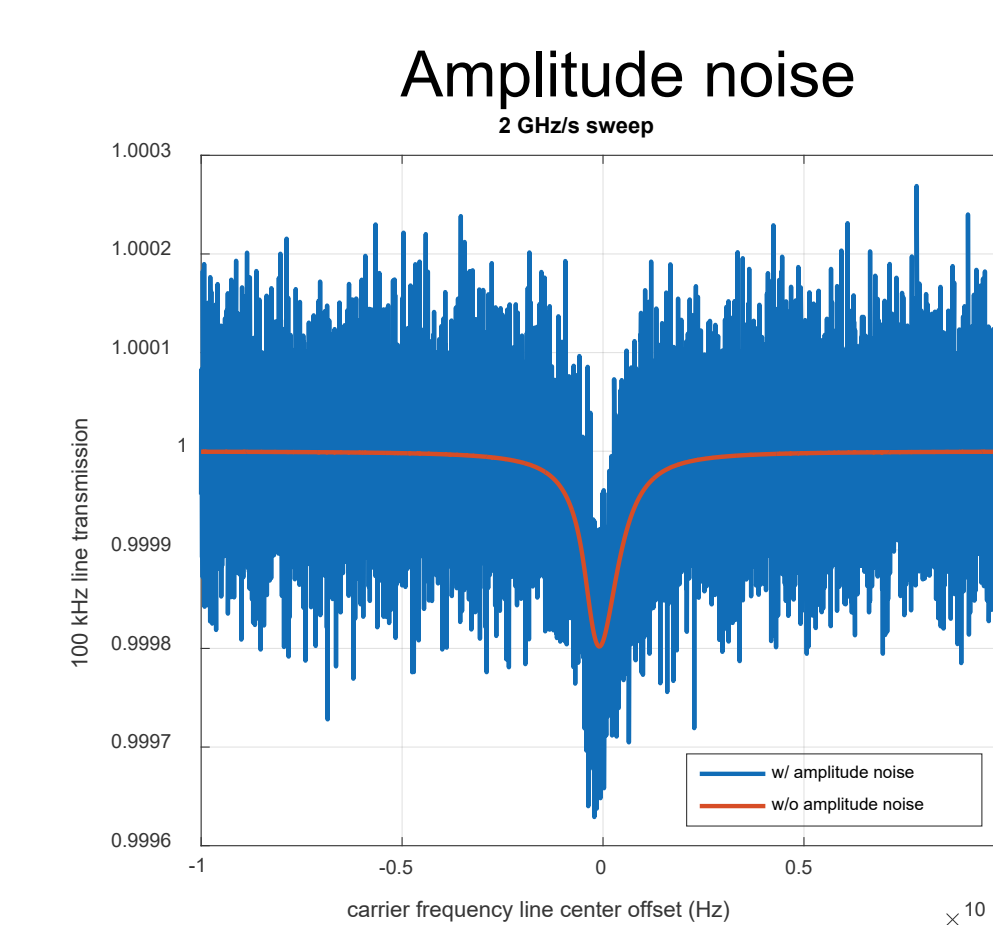
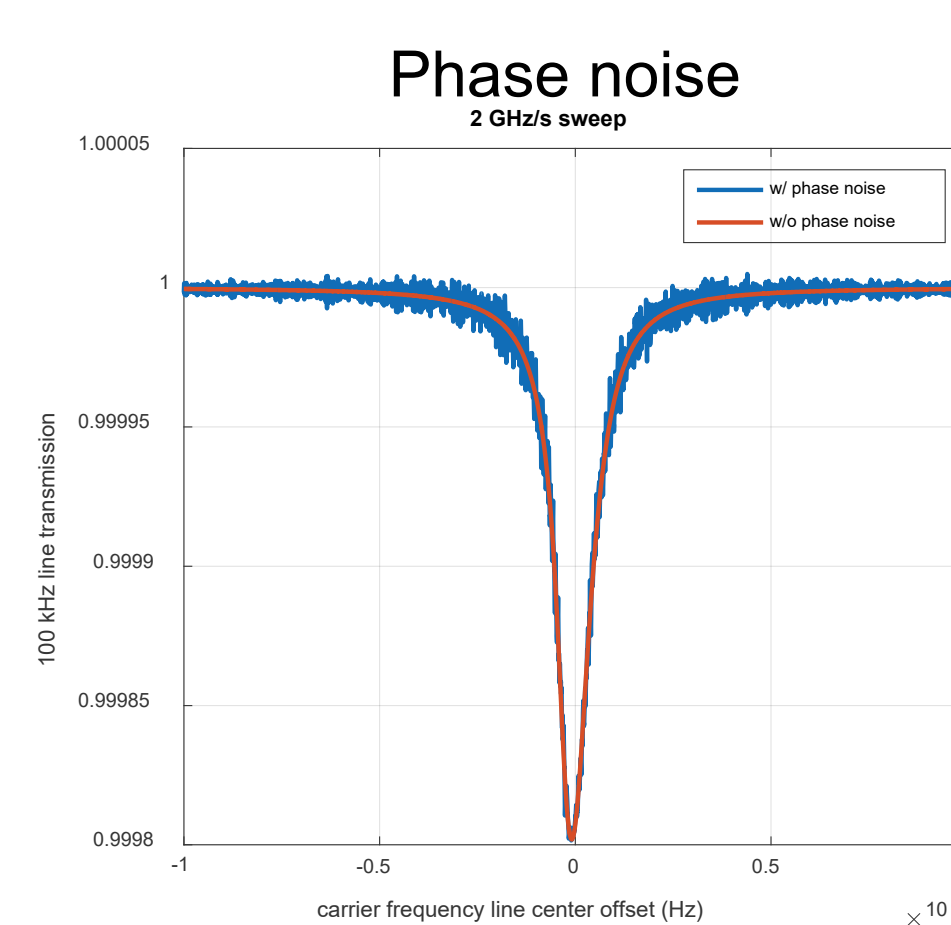
- One laser diode wavelength stabilization



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