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Terahertz absorption spectroscopy instrument for the detection of VOCs emitted by soil microorganisms

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Scientific context

Soil microorganisms release microbial volatile organic compounds (mVOCs) as intermediate or end products of their metabolism, that are also known as **metabolites**. Studying mVOCs emitted by soil into the air is thus a relevant way to assess its fertility and health. Because most of mVOCs are polar, **rotational spectroscopy** is a promising tool to fill the gaps in the analytical analysis of microbial activity.

Rotational spectroscopy

The rigid rotor solutions of the Schrodinger equation

$$\hat{H}Y_J^m(\theta, \phi) = E_J Y_J^m(\theta, \phi)$$

$$E_J = \frac{\hbar^2}{2I} J(J+1) \equiv BJ(J+1)$$

where $B = \frac{\hbar^2}{2I}$ is defined as the rotational constant for a given system. It is related to the moment of inertia I of a molecule.

<https://commons.wikimedia.org>

<https://doi.org/10.1109/JSEN.2012.2195487>

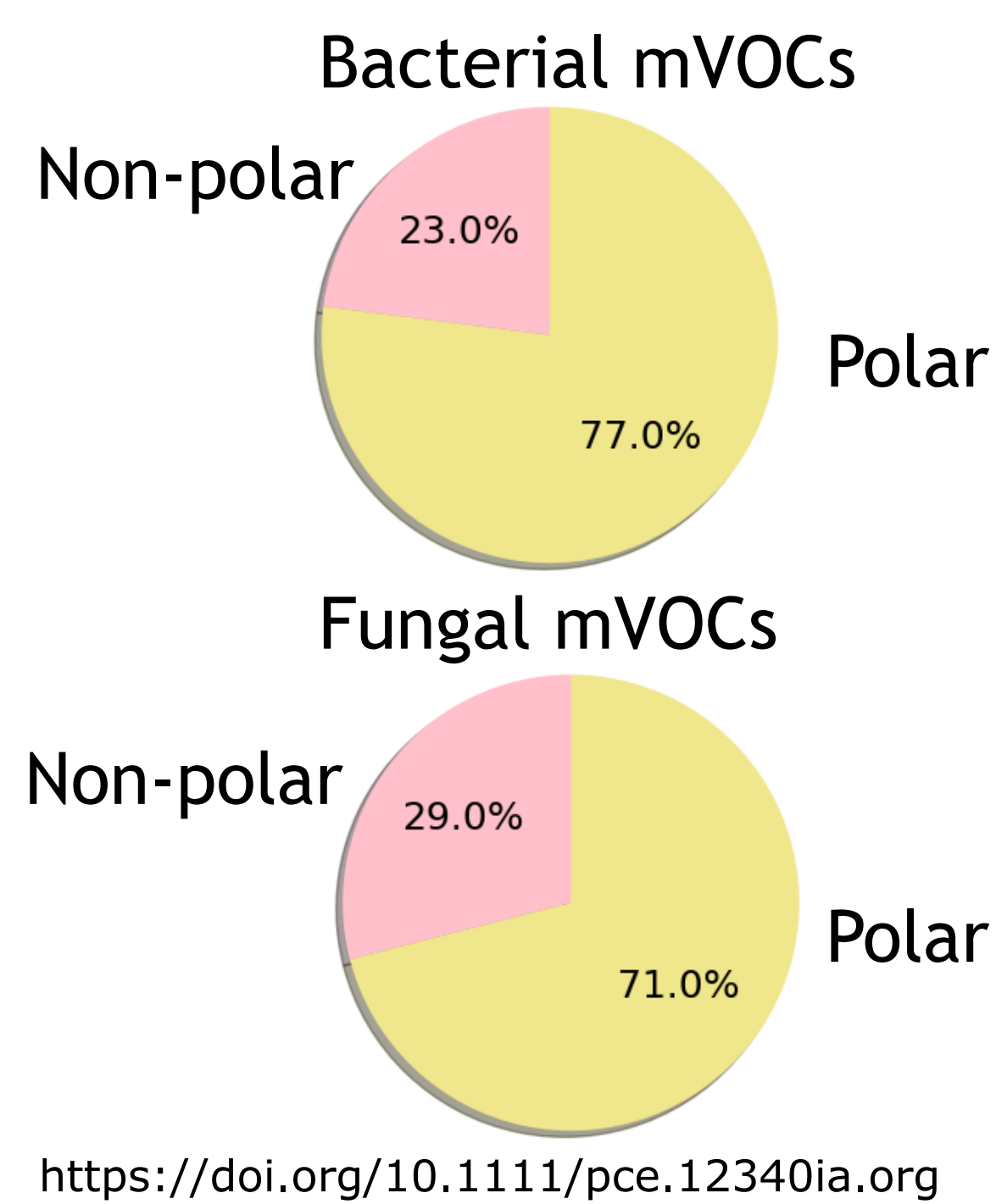
Can the rotational spectroscopy line up with other analytical techniques for detecting and analyzing mVOCs?

Rotational spectroscopy for mVOC detection

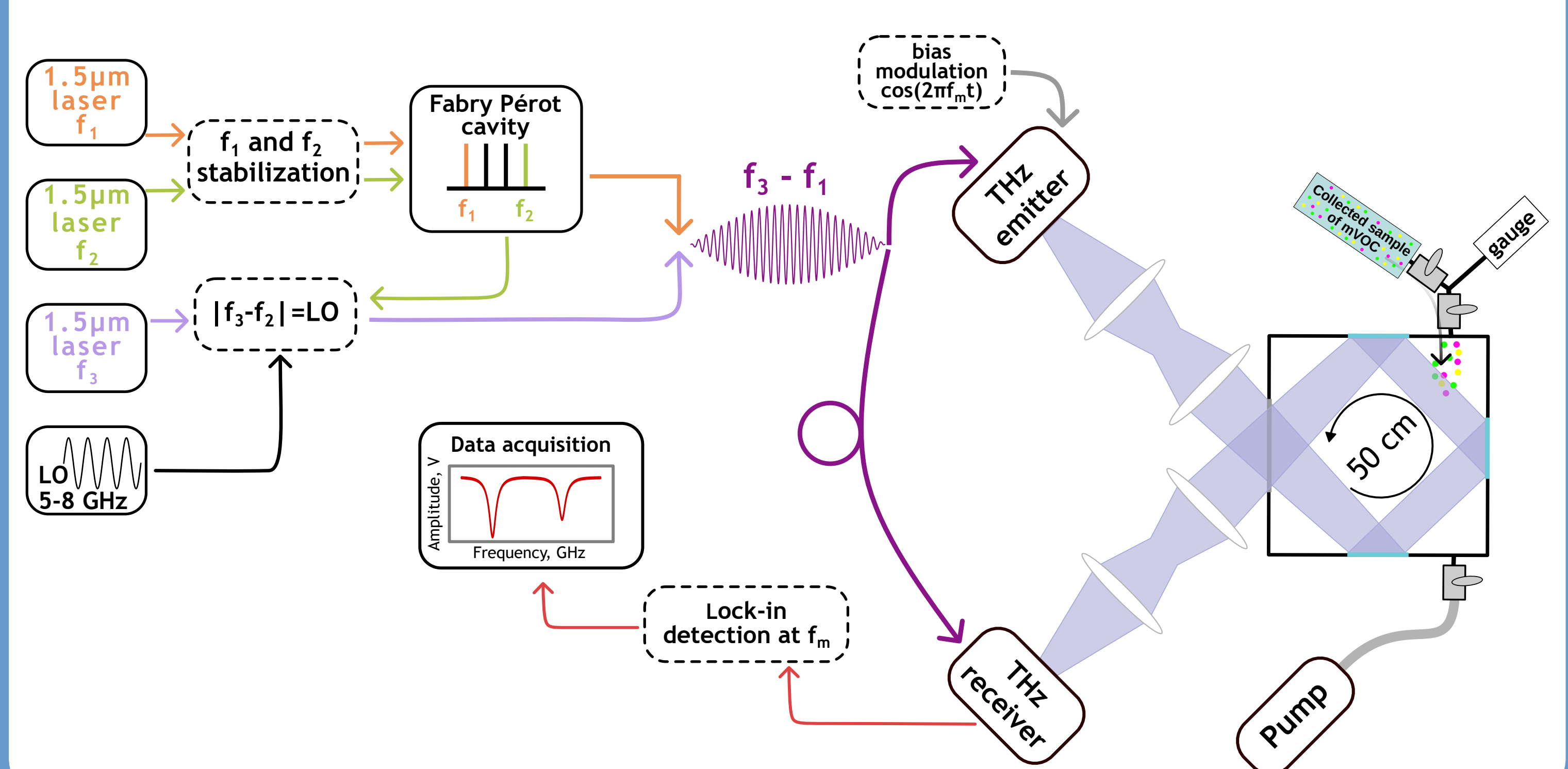
Rotational spectroscopy	Proton-transfer-reaction mass spectrometry (PTR-MS)
✓ no mass limit	✓ <i>In situ</i>
✓ frequency resolution 10 ² kHz	✓ 21-151 amu
✓ molecular integrity	✓ fast scan: 15 min
✓ non-ionizing radiation	✓ transportable
✗ slow scan: several hours long	✗ fragmentation
✗ <i>Ex situ</i>	✗ metabolites > 151 amu
✗ polar molecules	✗ proton affinity > water

✓ - advantage ✗ - limitation

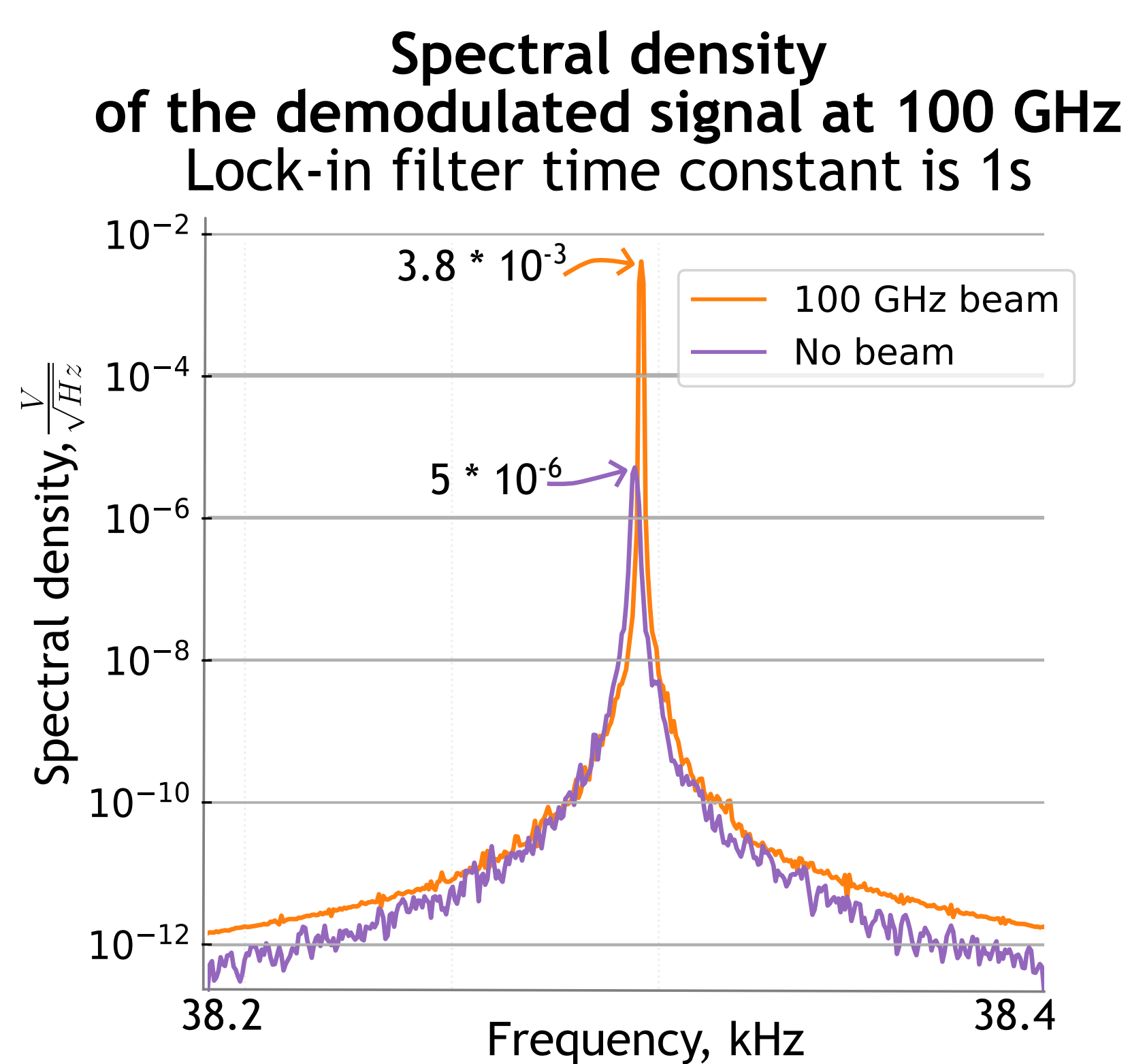
Rotational spectroscopy can be used to detect heavy polar metabolites



Detection system design

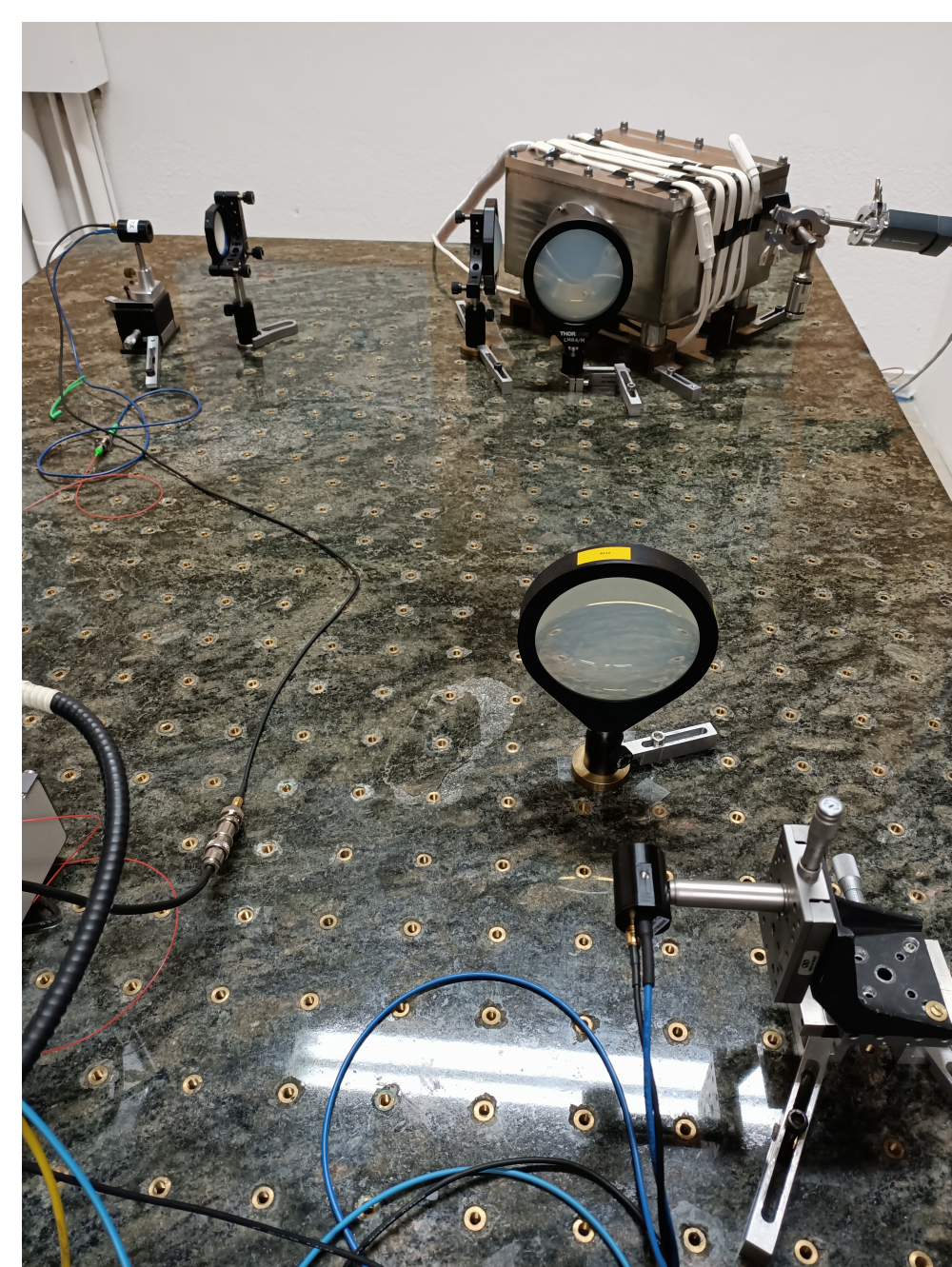


Detection system performance



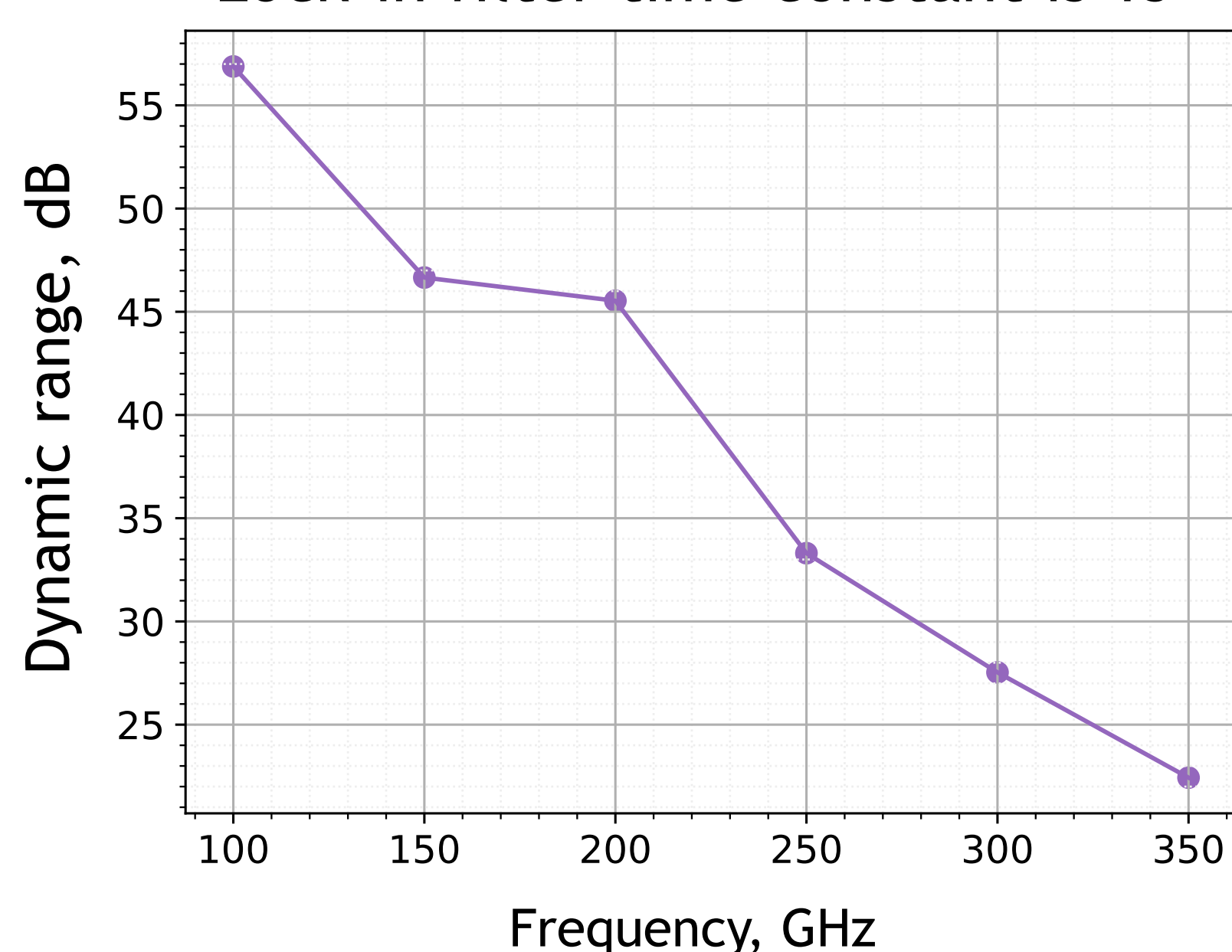
Vacuum system installation

Ultimate vacuum level:
6 * 10⁻³ mbar
Water outgassing rate:
9.8 * 10⁻³ mbar/h

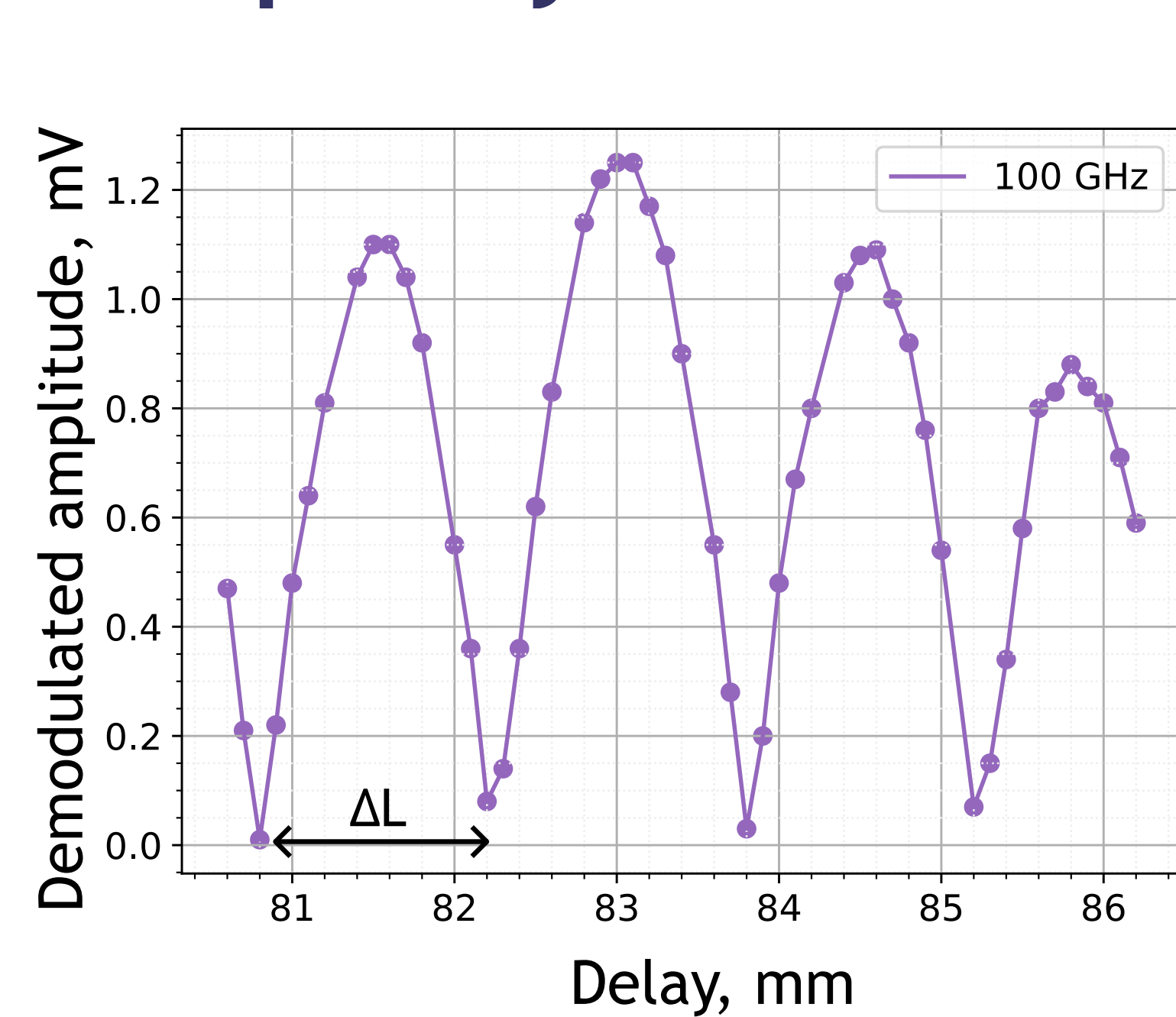


Dynamic range of the demodulated signal

Lock-in filter time constant is 1s



Frequency verification



Delay - difference in the optical propagation path between transmission and reception

$$\Delta L \sim \lambda$$

Set frequency	Estimated frequency
100 GHz	102 ± 3 GHz
150 GHz	154 ± 6 GHz
220 GHz	227 ± 9 GHz

The uncertainty will be reduced by adding measurements over a larger delay interval. Frequency calibration will be achieved by measuring the absorption spectrum of a known molecule.

Future prospects

- Study the detection limit of the system using acetonitrile (C₂H₃N) as a model for soil mVOCs.
- Demonstrate heavy polar metabolites detection:
 - Camphor C₁₀H₁₆O (152 amu)
 - Benzophenone C₁₃H₁₀O (182 amu)
 - Methyl salicylate C₈H₈O₃ (152 amu)
- Define a procedure for collecting mVOCs from a soil sample