

# *magnETHical*

MASTER THESIS: BUILDING A 25 MHZ NMR SPECTROMETER

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Maximilian Stabel

September 13, 2023

ETH Zürich

2023-09-13

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MASTER THESIS: BUILDING A 25 MHZ NMR SPECTROMETER

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Maximilian Stabel  
September 13, 2023  
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*“What I cannot create, I do not understand”*

—Richard Feynman

1

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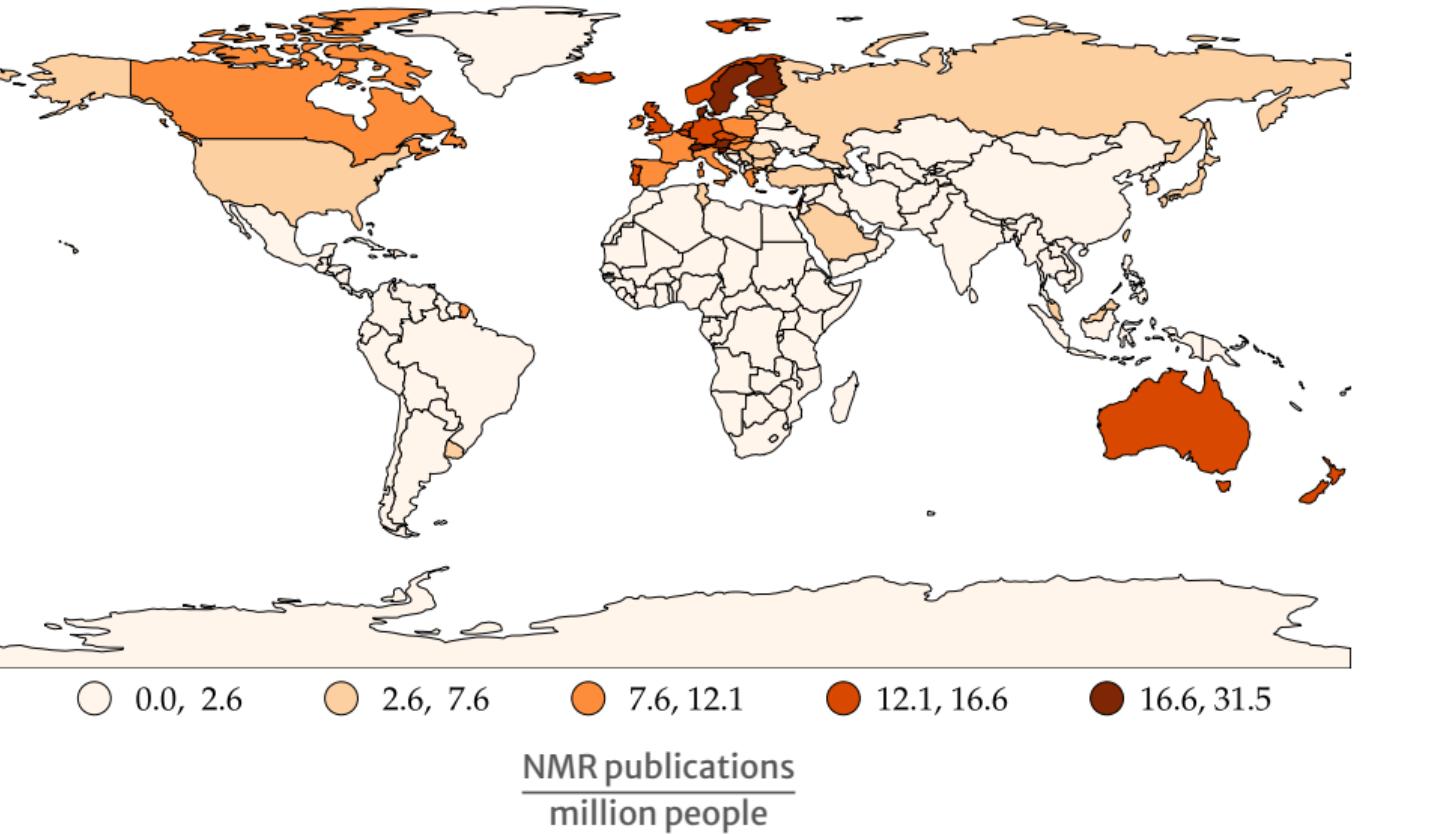
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*“What I cannot create, I do not understand”*

—Richard Feynman

1. In the spirit of Richard Feynman...
2. My master thesis is about building an NMR spectrometer
3. I'm Max and I'll be your host for today
4. Speaking of understanding...

There is not a lot of NMR research in the Global South



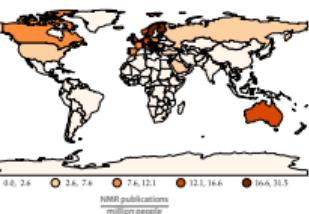
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There is not a lot of NMR research in the Global South

Reminder: What is NMR spectrometer

There is not a lot of NMR research in the Global South



# Nuclear Magnetic Resonance

- Nuclei absorb radio waves at a certain frequency when inside a magnetic field
- The nuclei emit radio waves at that same frequency when excited this way
- $f \sim B_0$  and surroundings

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## └ Nuclear Magnetic Resonance

- You: Understanding for own experiments
- The better we know the better we can use
- Push NMR development — better machines
- Transition: if not about you personally — more globally: applications

- Nuclei absorb radio waves at a certain frequency when inside a magnetic field
- The nuclei emit radio waves at that same frequency when excited this way
- $f \sim B_0$  and surroundings

## NMR is used across various fields

- Research (Structure Analysis, Drug Discovery, ...)
- Medicine (Imaging, Diagnosis, ...)
- Industry (Process Control, Drug screening, ...)
- Education (Quantum Mechanics, Quantum Computing, ...)

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└ NMR is used across various fields

## 1. Some of you already know, but here are some reasons why NMR is useful

- Research (Structure Analysis, Drug Discovery, ...)
- Medicine (Imaging, Diagnosis, ...)
- Industry (Process Control, Drug screening, ...)
- Education (Quantum Mechanics, Quantum Computing, ...)

**Build an accessible  
NMR spectrometer**

- 1. The goal of my thesis was...**

Preview

The parts

The complete setup

Experimental Results

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└ Preview

The parts

The complete setup

Experimental Results

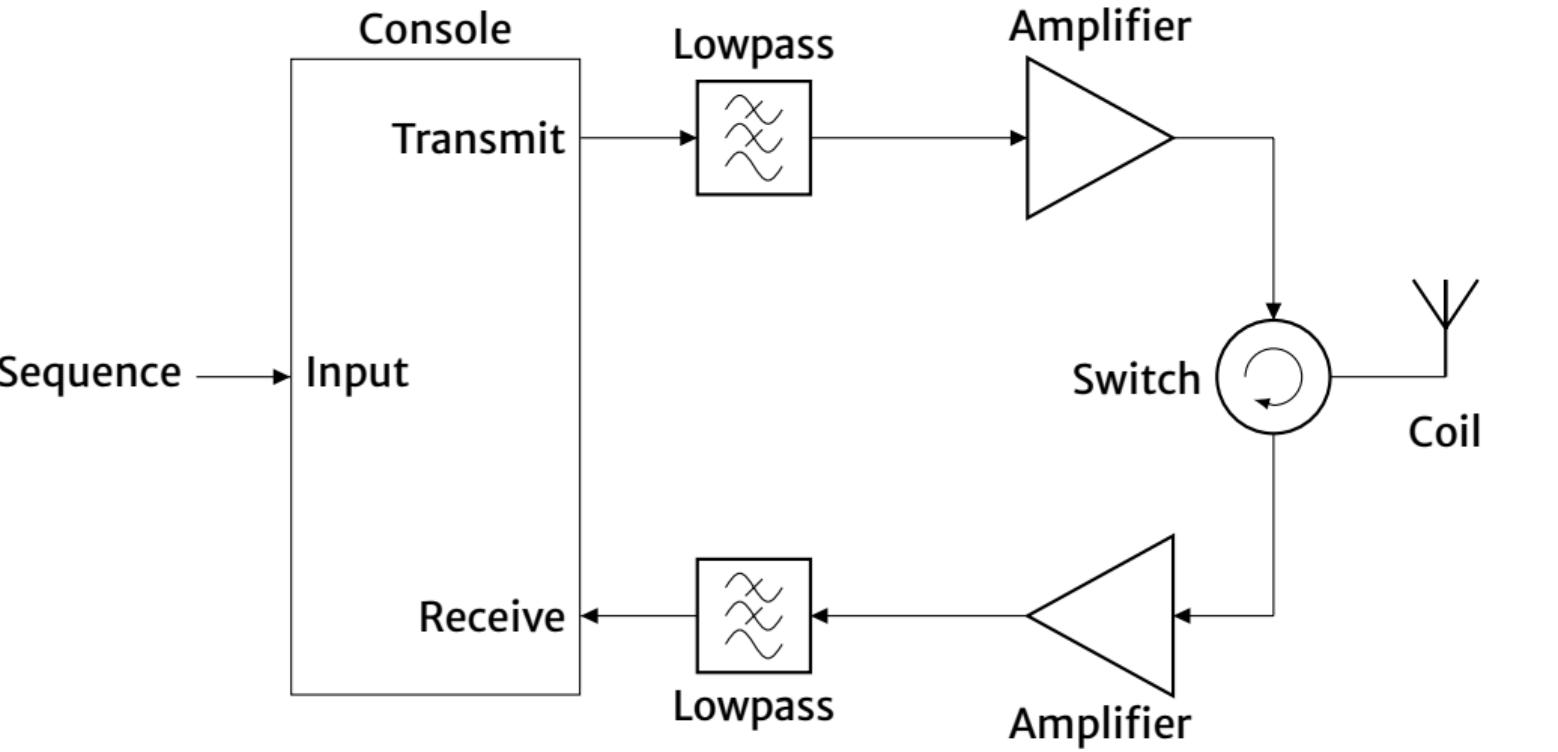
## THE PARTS

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THE PARTS

2023-09-13 *magnETHical*  
└ The parts

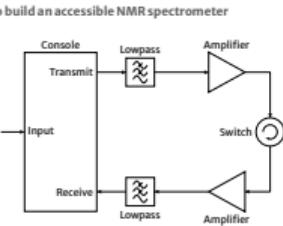
Our goal is to build an accessible NMR spectrometer



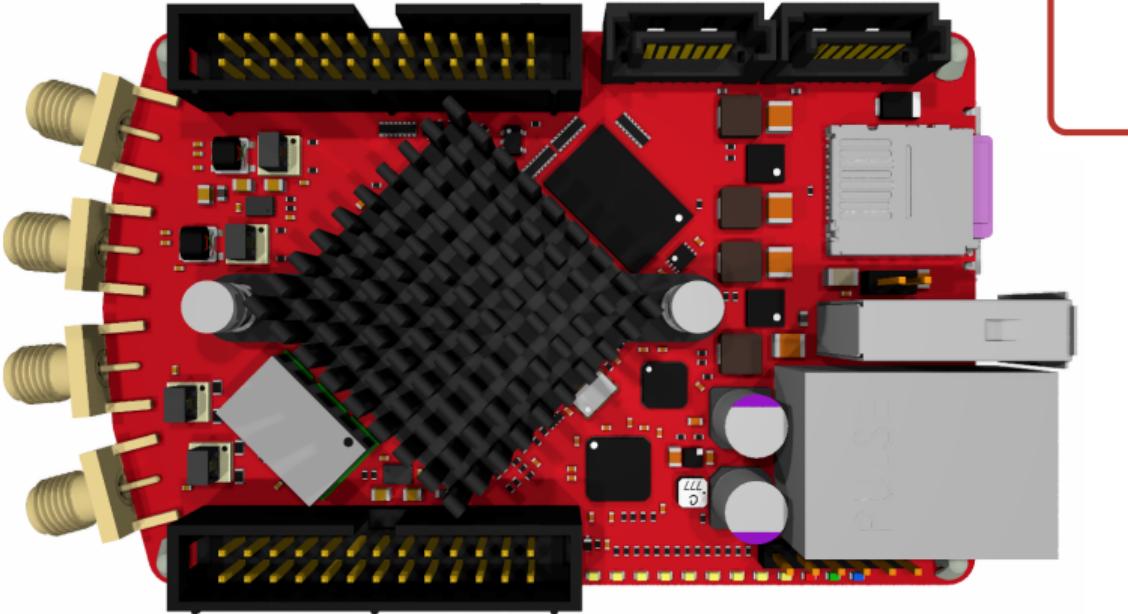
6

2023-09-13 **magnETHical**  
└ The parts

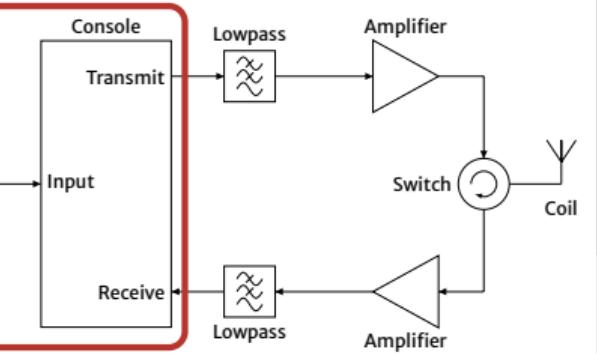
1. Go through the parts left to right
2. Our switch only, others might include more analog processing



The console  
is a ready-made FPGA board\*



\*Red Pitaya SDRlab 122-16



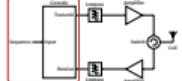
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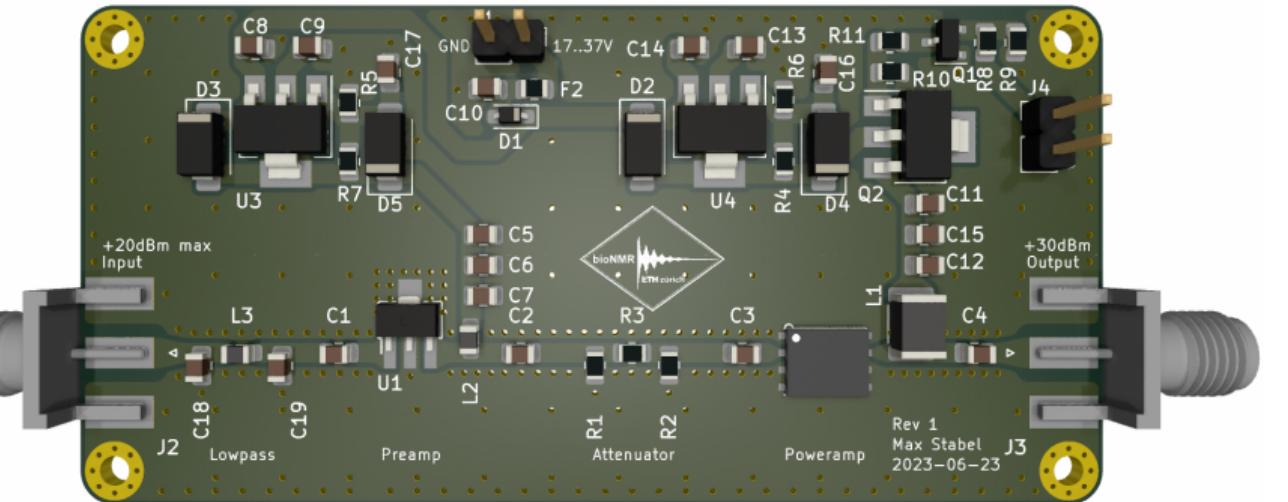
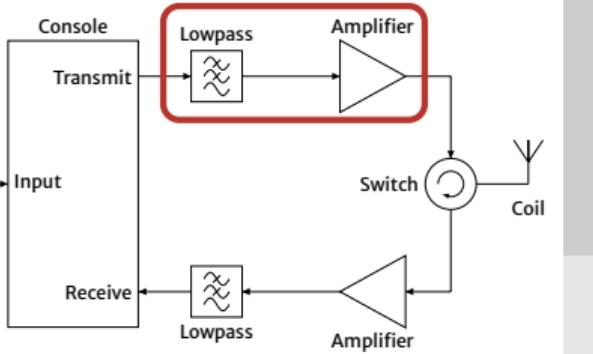
## The parts

FPGA, SDR, RF, Antenna, Power

1. FPGA == programmable hardware, very fast
2. oversampling
3. CIC filter (decimation, low pass filter, moving average)
4. The signal needs to be filtered and then amplified: Next Slide



The power amplifier has two stages

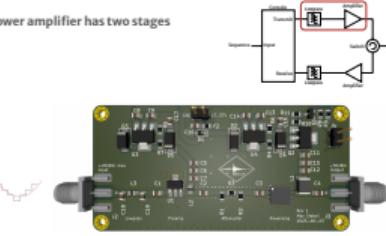


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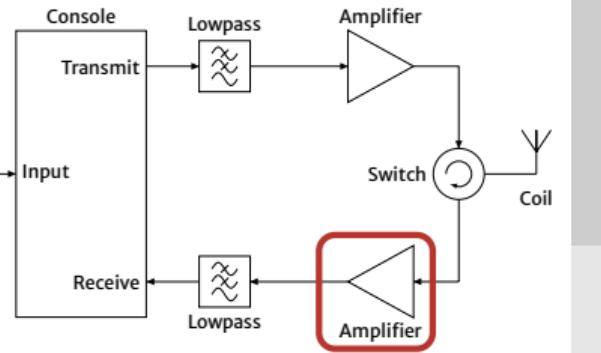
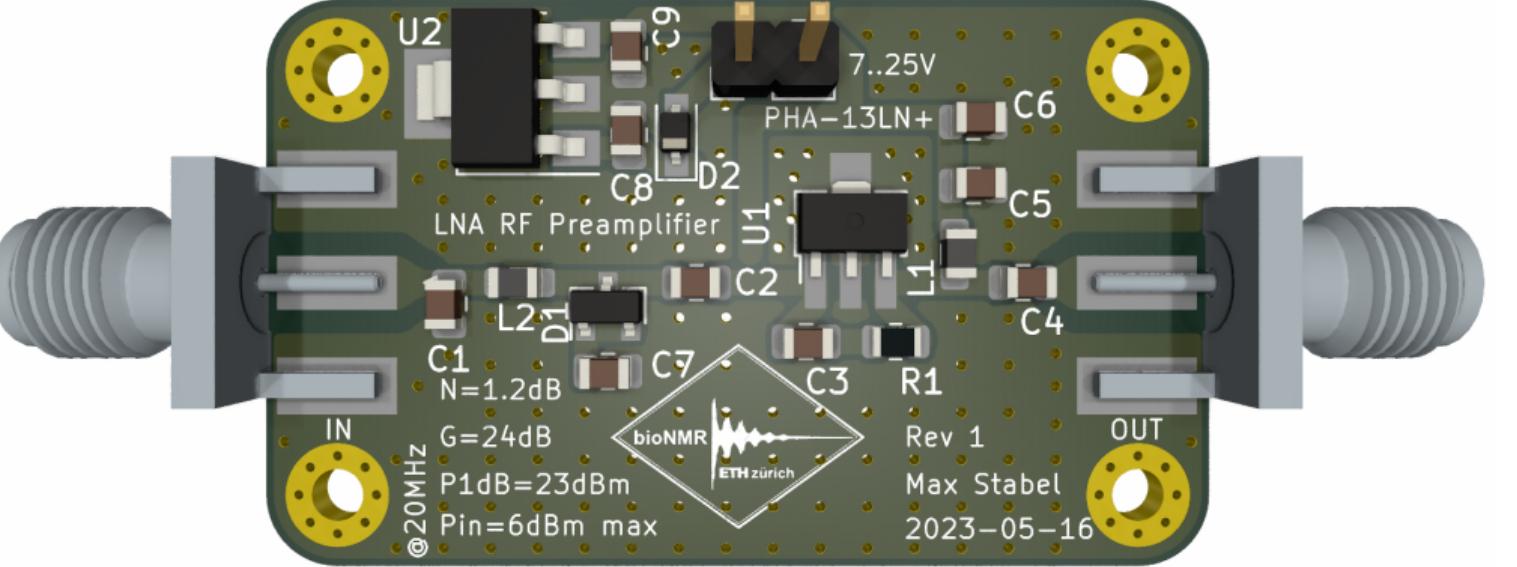
## The parts

1. We want cheap, so using a simple is the obvious first approach
2. Unfortunately there's a lot to do:
  - Input/Output Impedance Matching
  - Bias Tee
  - DC coupling
  - stability calculations
  - feedback
  - temperature compensation (current feedback)
3. A complete amplifier is quite expensive
4. Solution: Use monolithic (integrated) amplifier
5. Take care of heat dissipation (Class-A)
6. dB is logarithmic unit



The power amplifier has two stages

The low-noise amplifier had instability issues

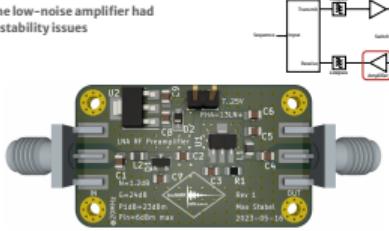


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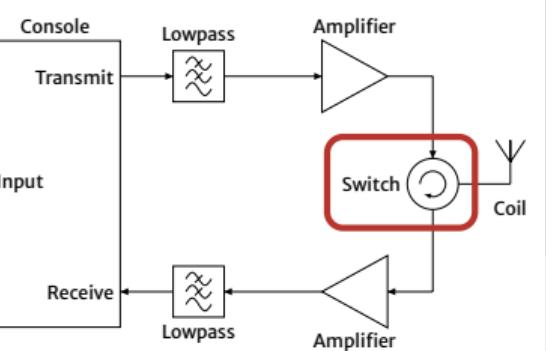
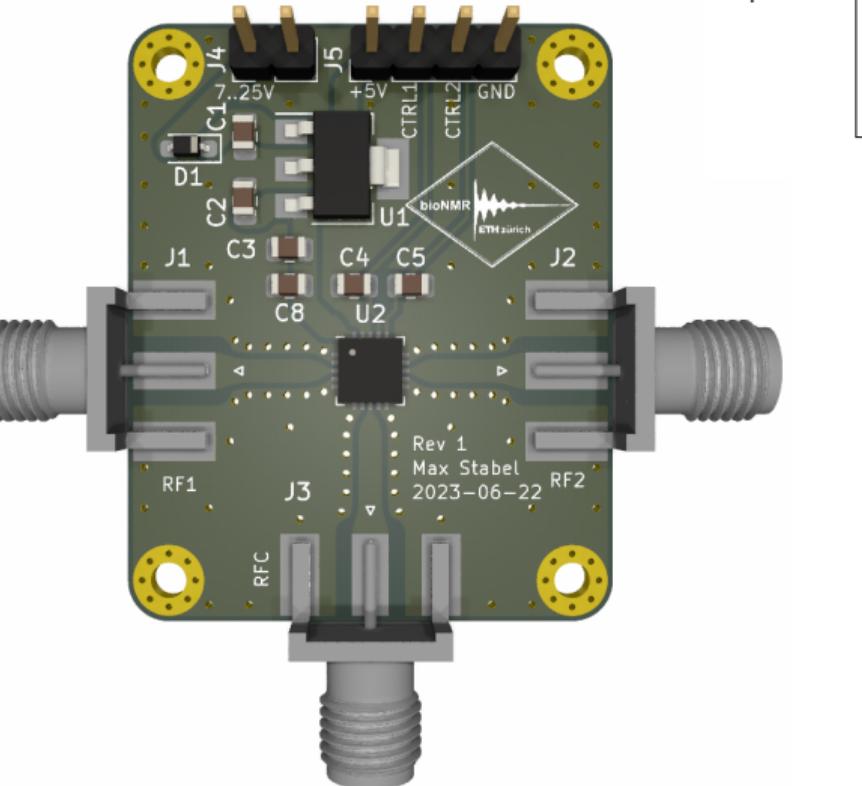
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## The parts

1. Low-noise
2. Feedback loop — stray capacitance
3. Solution: Smaller housing, shorter loop
4. We need 3x for enough gain



**We use a transistor-based active switch**



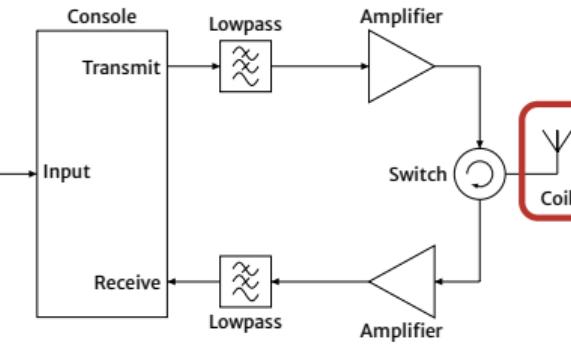
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## The parts

1. Active
  2. Isolation: 60 dB
  3. Silicon-on-insulator (not pHEMT GaAs) i.e. FET tech, not PIN-Diode
  4. PIN-Diode switch also possible, but
    - usually higher leakage
    - slower switching
    - harder to integrate on a chip
    - but higher power capabilities

## The probe

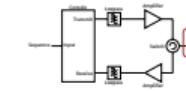


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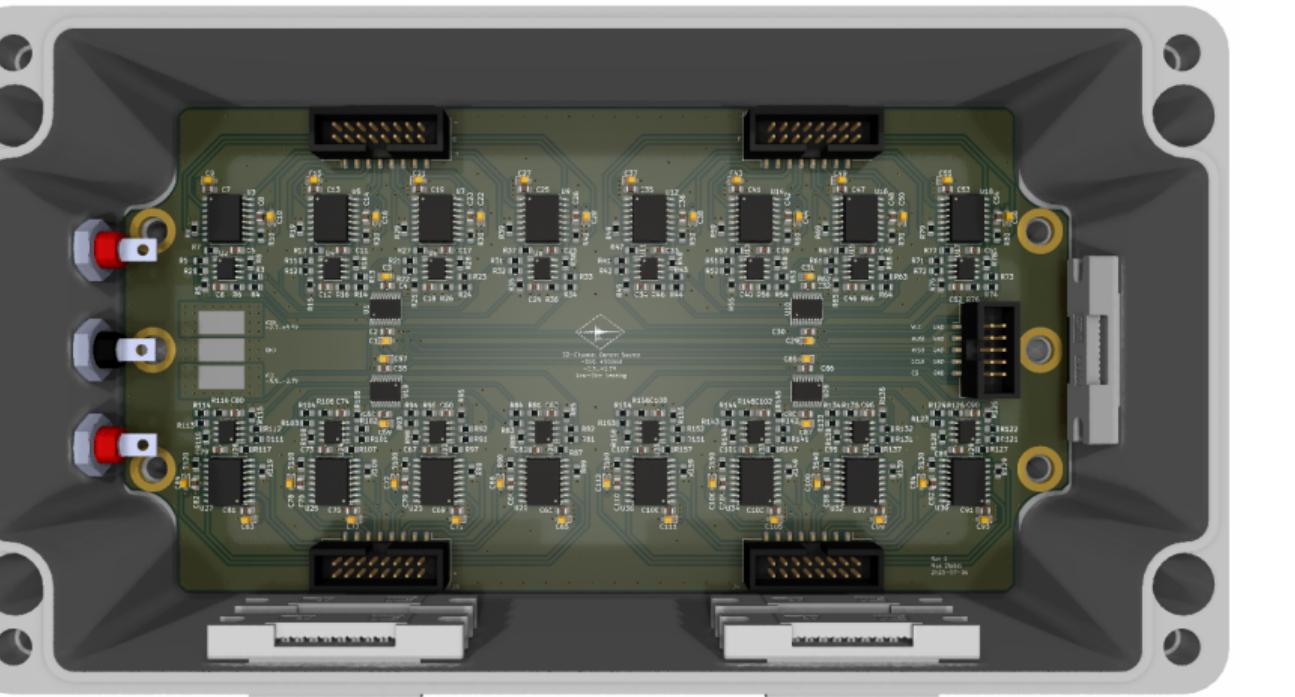
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## The parts

1. Many turns — high inductance — low capacitance — sensitive to stray capacitance



**A 32-channel current supply is designed but untested**



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## The parts

Accessed from <http://www.industrydocuments.ucsf.edu/docs/ajhs0001>



All current supply is designed but untested

## THE COMPLETE SETUP

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└ The complete setup

THE COMPLETE SETUP

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Our NMR is affordable ...

	600 MHz <sup>†</sup>	mini-circuits	<i>magnETHical</i>
Power Amplifier	50 000	323.49	36.01
Switch	-	82.06	20.05
Probe	100 000	-	≈15.00
Low-Noise Amplifier	50 000	409.38	73.11
Shim Driver	-	-	257.08
Console	200 000	-	662.53
Magnet	1 000 000	-	≈9000.00
<b>Sum</b>			<b>10 142.80</b>

<sup>†</sup>estimated costs

Prices incl. VAT [CHF]

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## The complete setup

↓ NMR console

	600 MHz <sup>†</sup>	mini-circuits	<i>magnETHical</i>
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Prices incl. VAT [CHF]

... competitive ...

	Superconducting	Benchtop	<i>magnETHical</i>
Price [k CHF]	200–18 000	50–150	≈10
Frequency [MHz]	300–1200	40–125	25
Resolution [Hz]	≈0.2	0.2–1	≈2.5/50 <sup>†</sup>
Weight [kg]	600–15 000	25–150	≈5

<sup>†</sup>with/without shims

For 5mm standard NMR tubes

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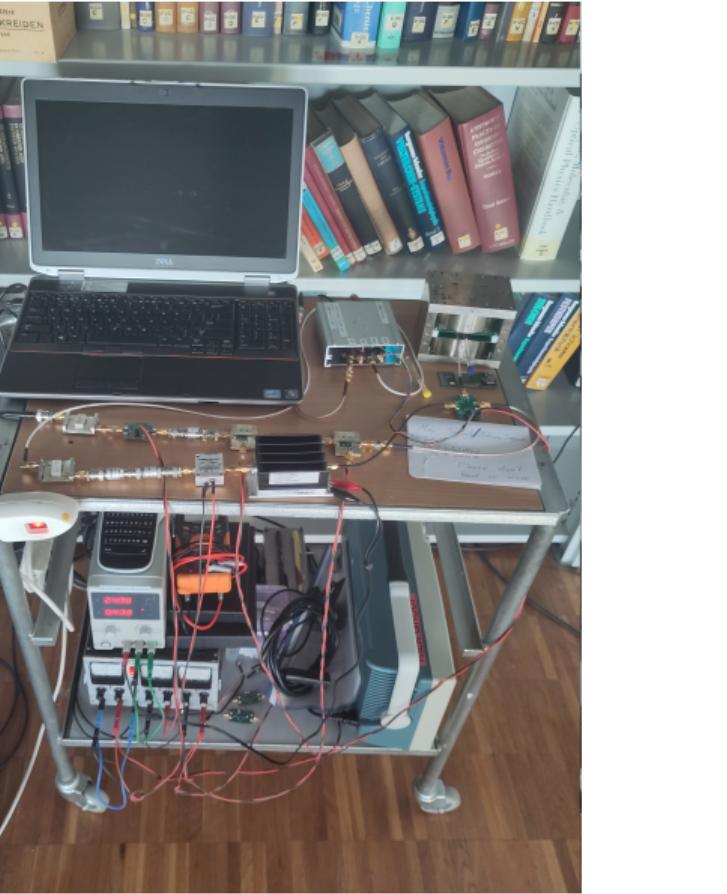
The complete setup

... competitive ...

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<sup>†</sup>with/without shims  
For 5mm standard NMR tubes

... and portable



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## └ The complete setup



## EXPERIMENTAL RESULTS

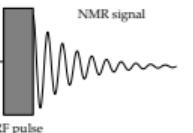
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EXPERIMENTAL RESULTS

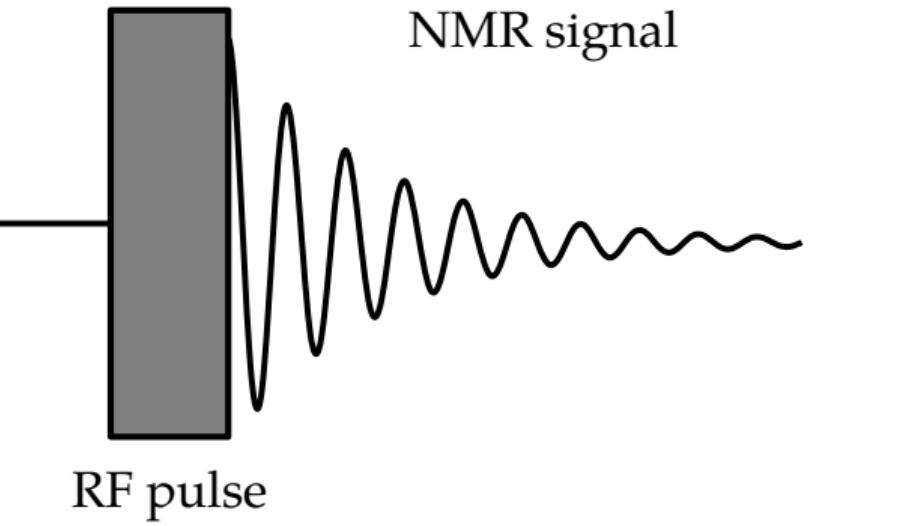
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## └ Experimental Results

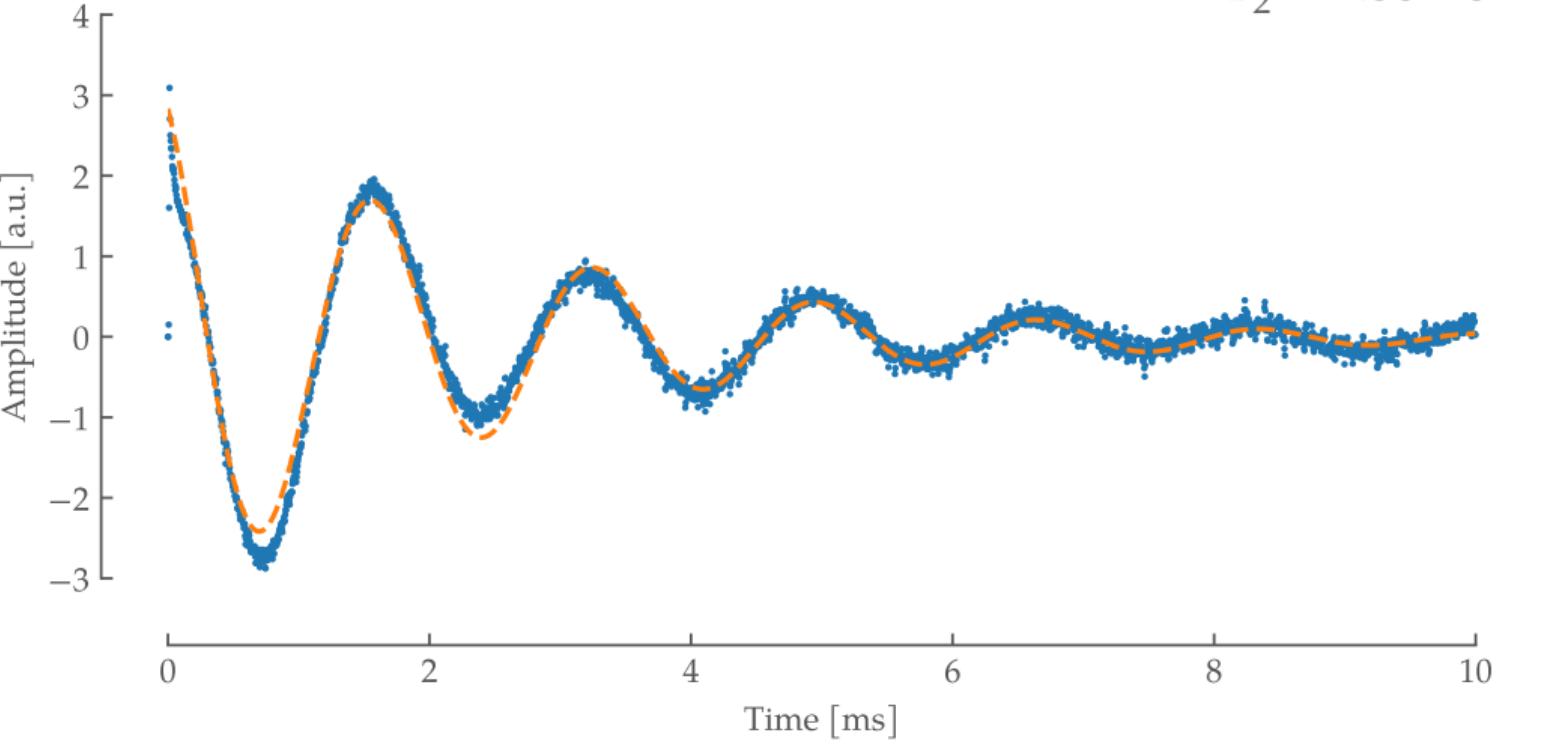
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## Simple Pulse Sequence



We can already see a water FID

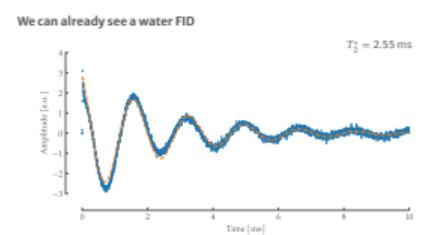


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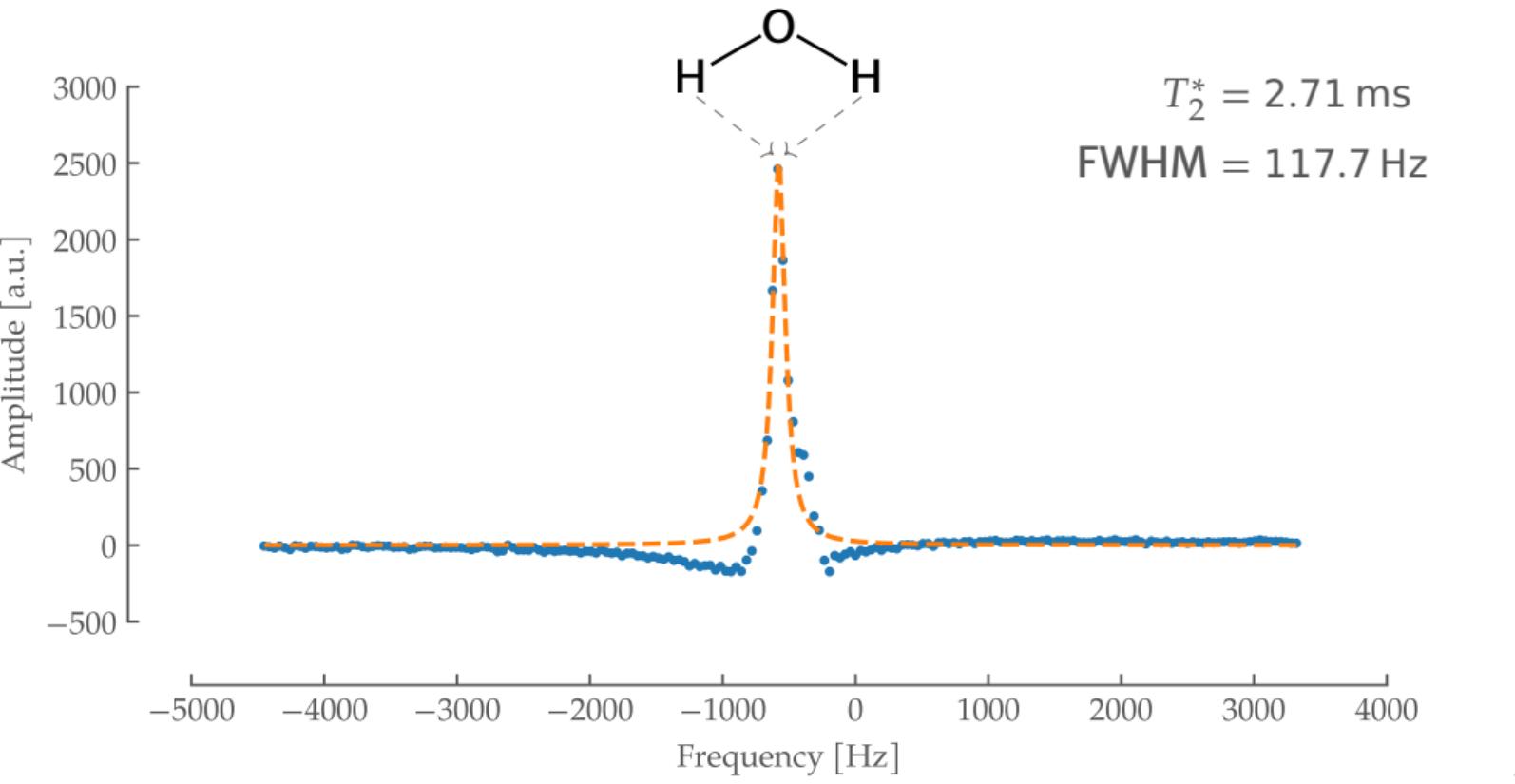
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## └ Experimental Results

1. Outliers at the beginning are due to CIC filters



...and do a Fourier transform

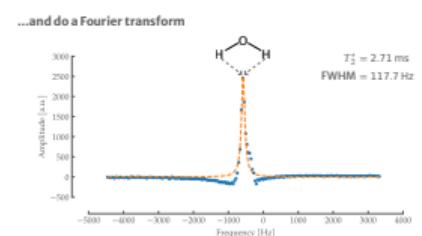


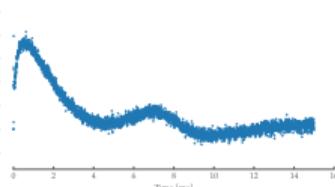
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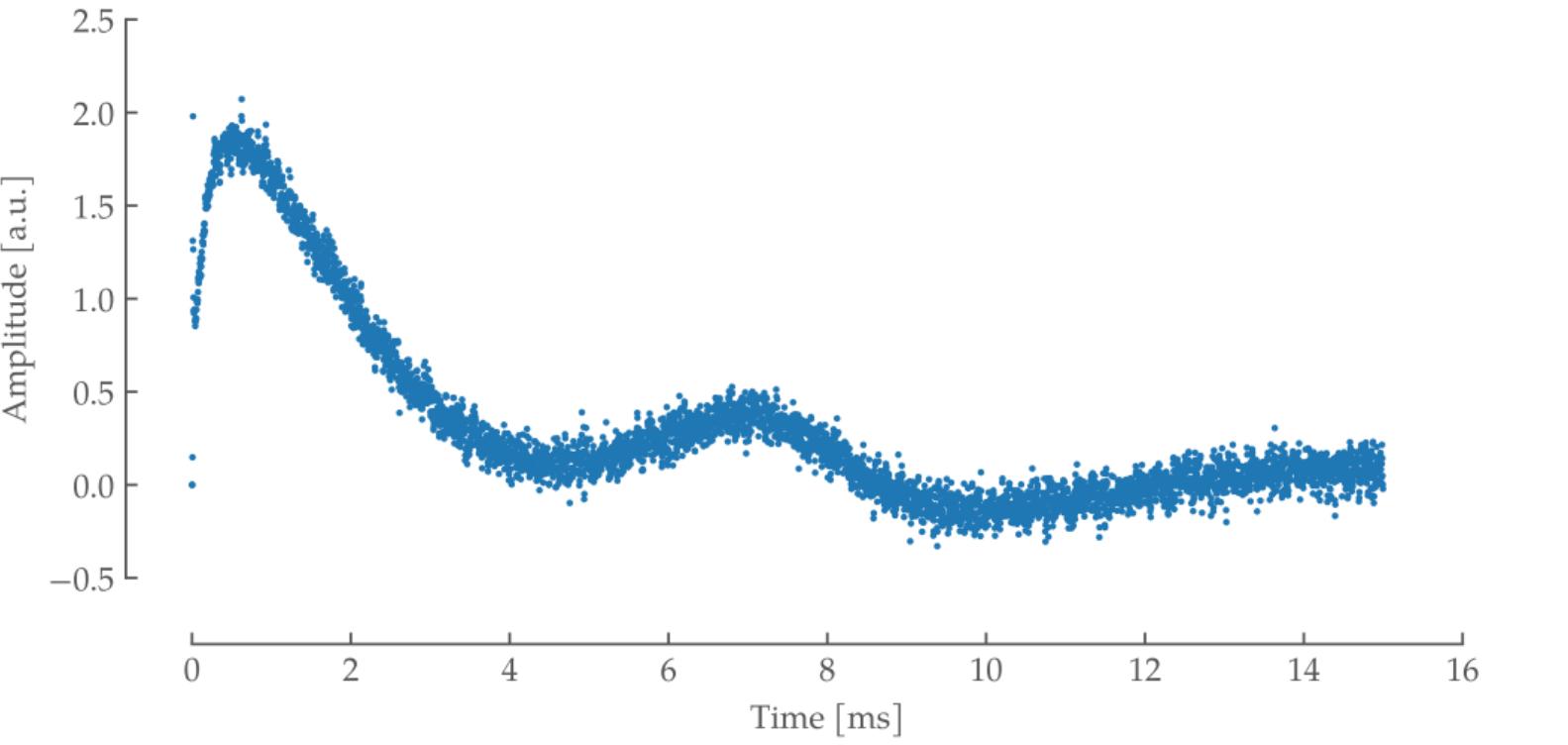
## └ Experimental Results

1. Not Lorentz because of missing shimming/inhomogeneities
2. Measured input signal of -92dBm/15.8uV resulted in amplitude of 2200
3. SNR of around 350, With FWHM 2.5Hz/1ppm we estimate snr of 11000





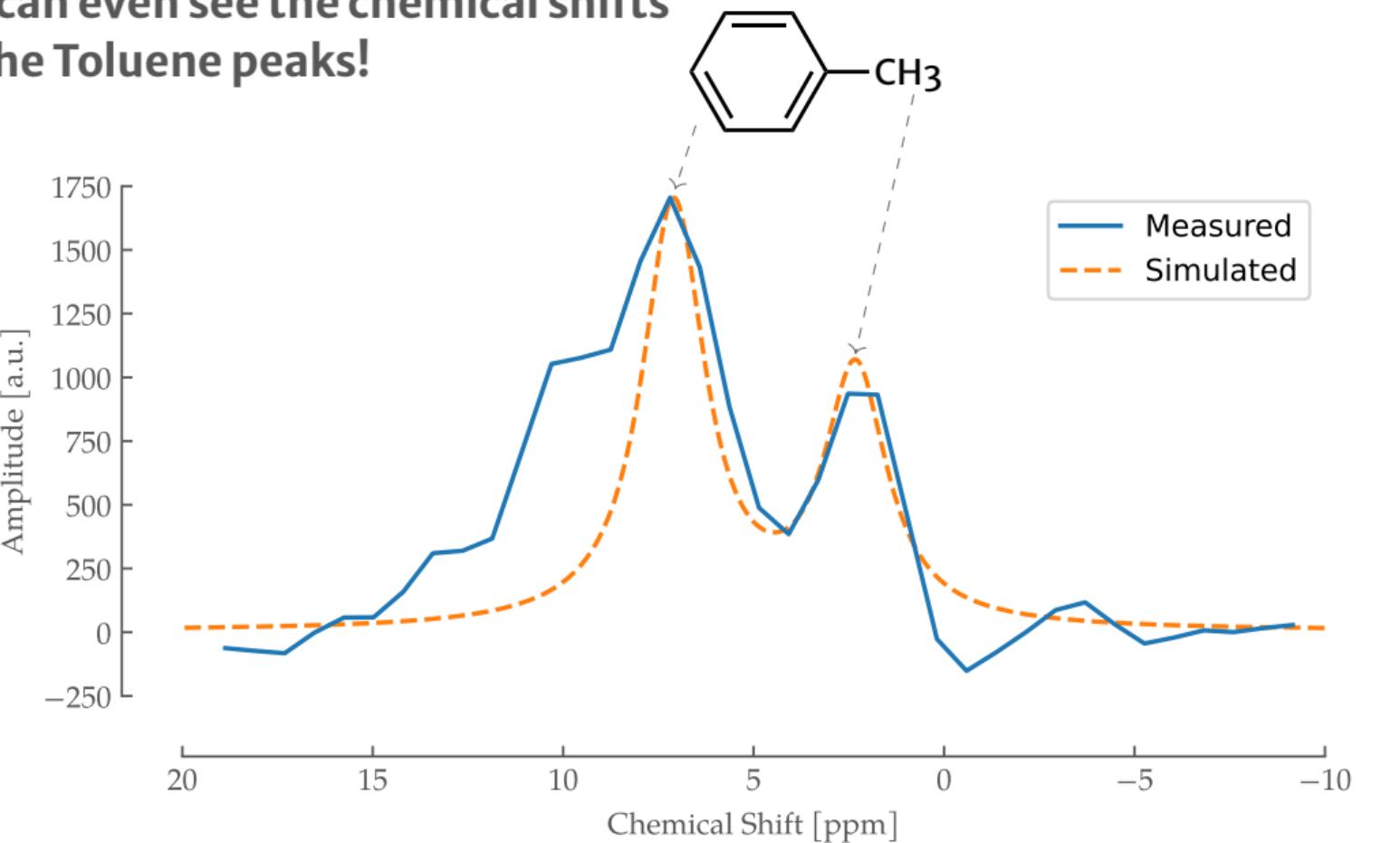
Toluene also has a visible signal



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## └ Experimental Results

We can even see the chemical shifts  
of the Toluene peaks!



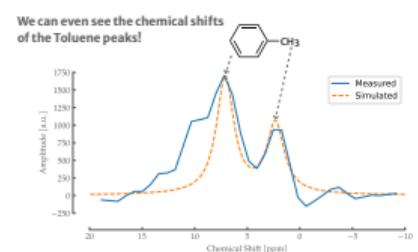
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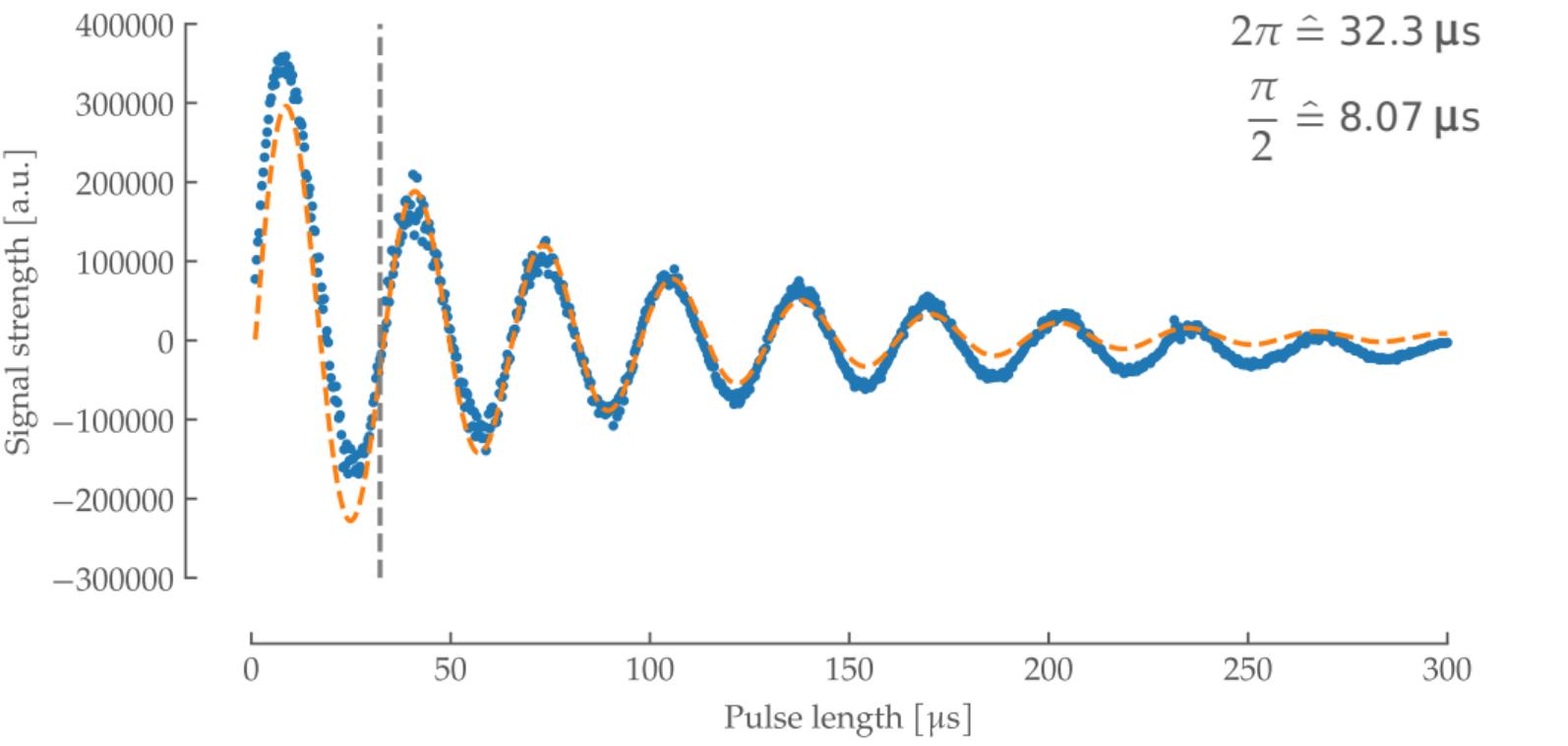
## └ Experimental Results

It's a full tube of toluene, not a solution

1. Reasons for sidepeak: no apodization (truncation of FID), no shimming, inhomogeneities/not centred



## Rabi nutation (pulse calibration) of water



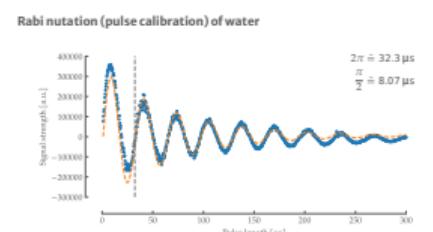
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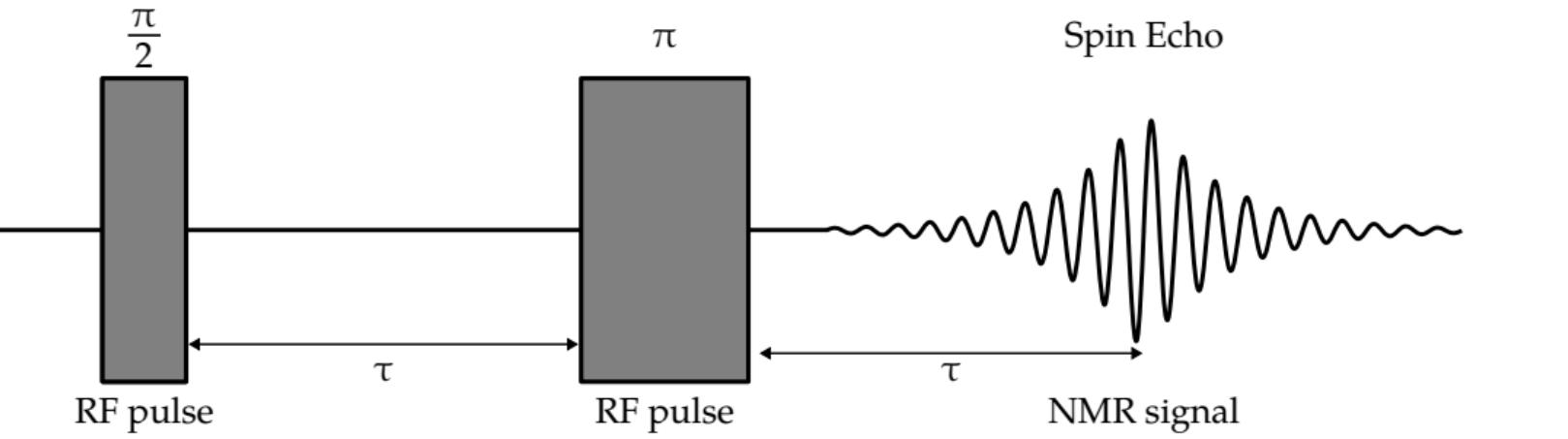
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## └ Experimental Results

1.  $T_{\text{period}} = 32 \mu\text{s}$
2.  $T_{\frac{\pi}{2}} = 8 \mu\text{s}$



## Spin Echo Sequence

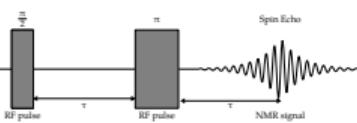


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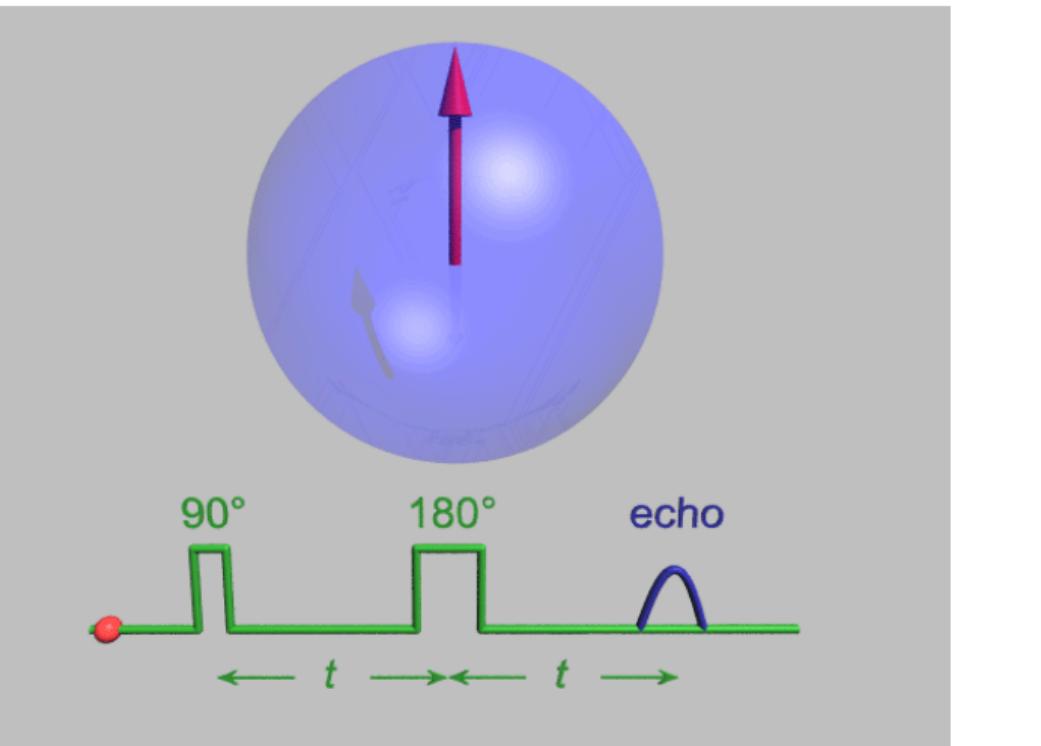
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## └ Experimental Results

Spin Echo Sequence



# Spin Echo Animation

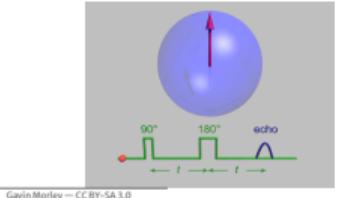


Gavin Morley — CC BY-SA 3.0

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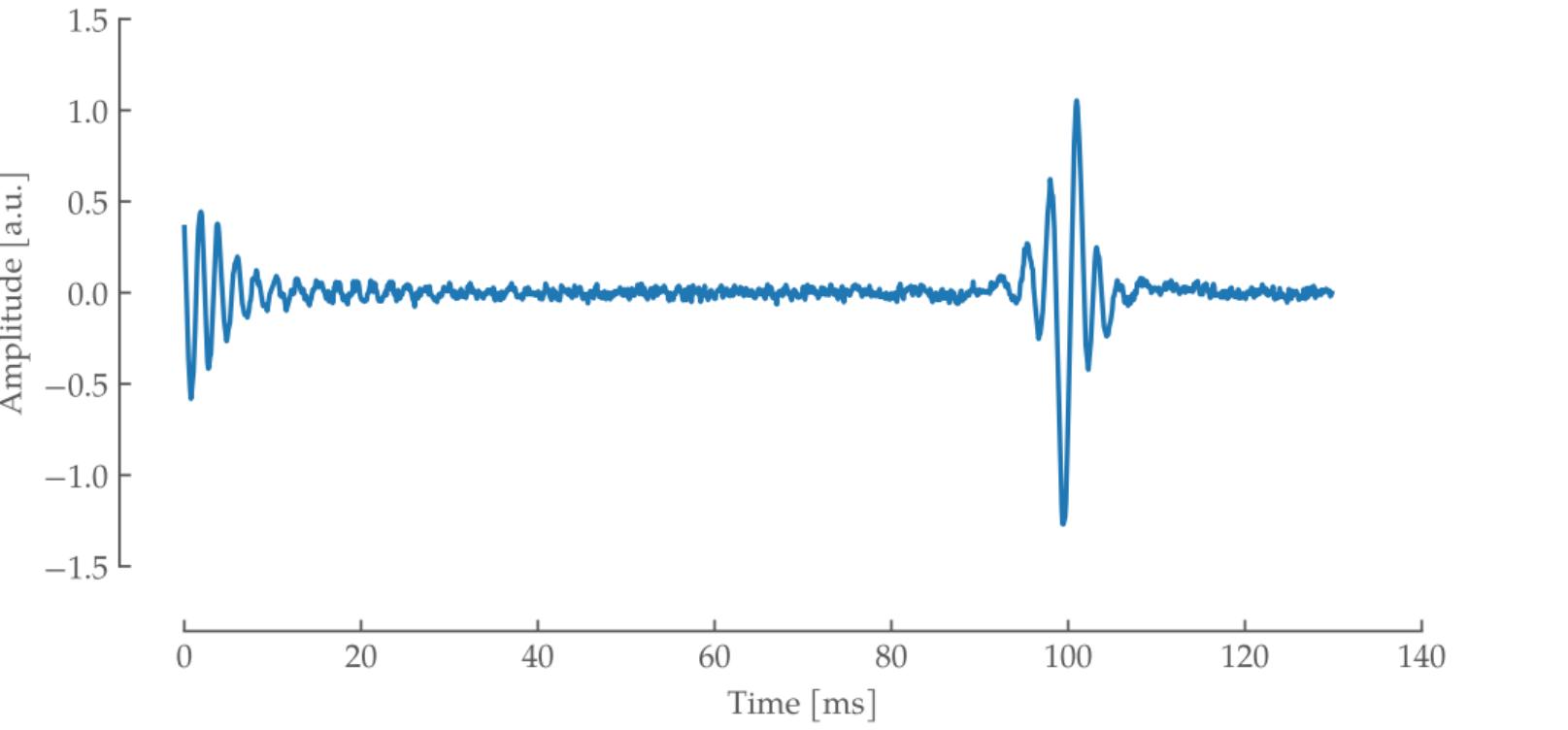
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## └ Experimental Results



Gavin Morley — CC BY-SA 3.0

## Spin Echo Measurement

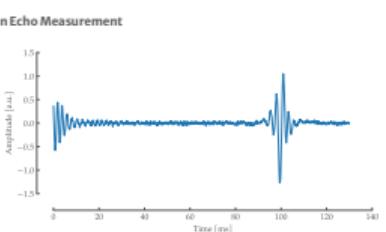


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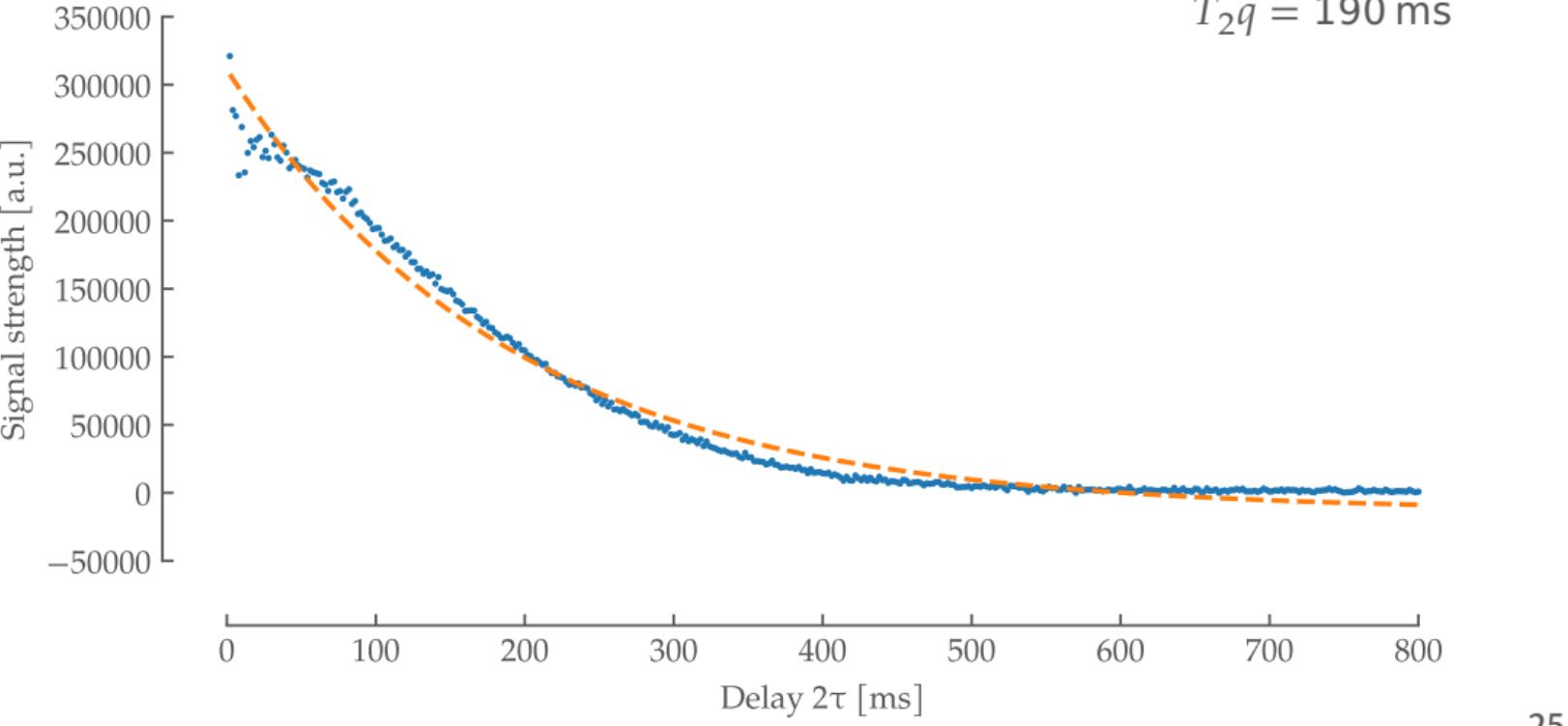
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## Experimental Results



## $T_2$ decay of water



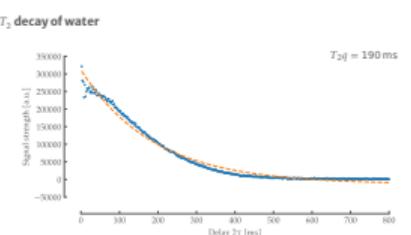
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## └ Experimental Results

1.  $T_2 =$



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## └ Experimental Results

Demo time!

## Review

- Why?
- The parts
  - Console
  - Amplifiers
  - Switch
  - Probe

- Capture & Process Software
- Experimental Results
- Demonstration

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## └ Experimental Results

- Why?
- The parts
  - Console
  - Amplifiers
  - Switch
  - Probe
- Capture & Process Software
- Experimental Results
- Demonstration

## Outlook

- Shim Driver
- Shielding
- Improve any part individually
  - Cheaper Magnet
  - Better Probe
  - Software (CIC compensation filter, frequency adjustment during pulse, ...)
- Investigate temperature stability
- Sell it to NexMR (or do Photo-CIDNP ourselves)

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## Experimental Results

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*“I have not yet lost that sense of wonder, and of delight, that this delicate motion should reside in all ordinary things around us, revealing itself only to him who looks for it.”*

*“There the snow lay around my doorstep — great heaps of protons quietly precessing in the Earth’s magnetic field.”*

— E.M. Purcell

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## └ Experimental Results

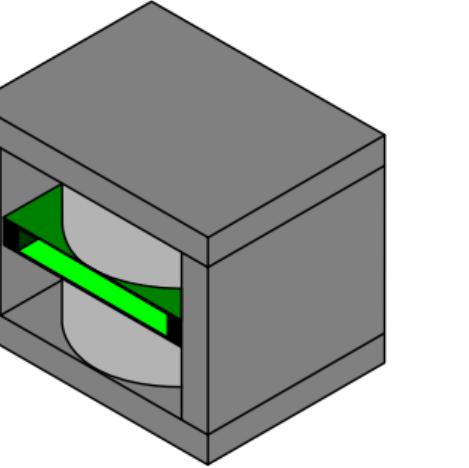
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— E.M. Purcell

1. Circling back to the beginning, I would like to end with a quote by E.M. Purcell
2. I wouldn’t have thought I would get a glimpse of this wonder that Purcell describes when starting my thesis here, but I’m glad I did.
3. And I hope none of you have lost it yet

Thank you!



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Find everything on



[https://gitlab.ethz.ch/mstabel/  
nmr-spectrometer](https://gitlab.ethz.ch/mstabel/nmr-spectrometer)

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## └ Experimental Results



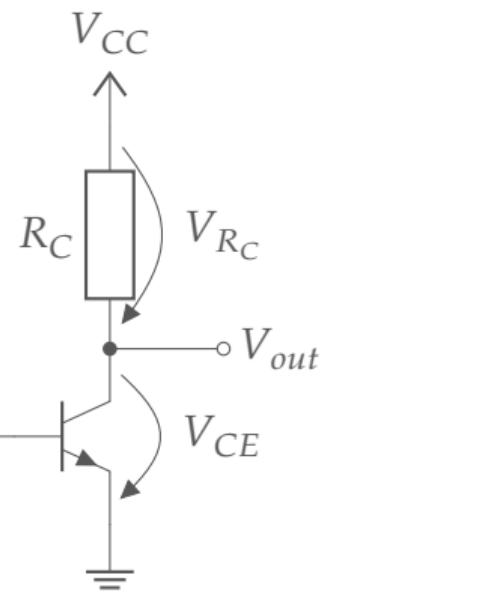
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**Backup**

# An amplifier is basically just a transistor

- Transistor:  
voltage-controlled current source
- higher voltage → higher current
  - higher voltage  $V_{R_C}$
  - lower voltage  $V_{CE}$
  - 180° phase shift

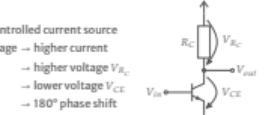


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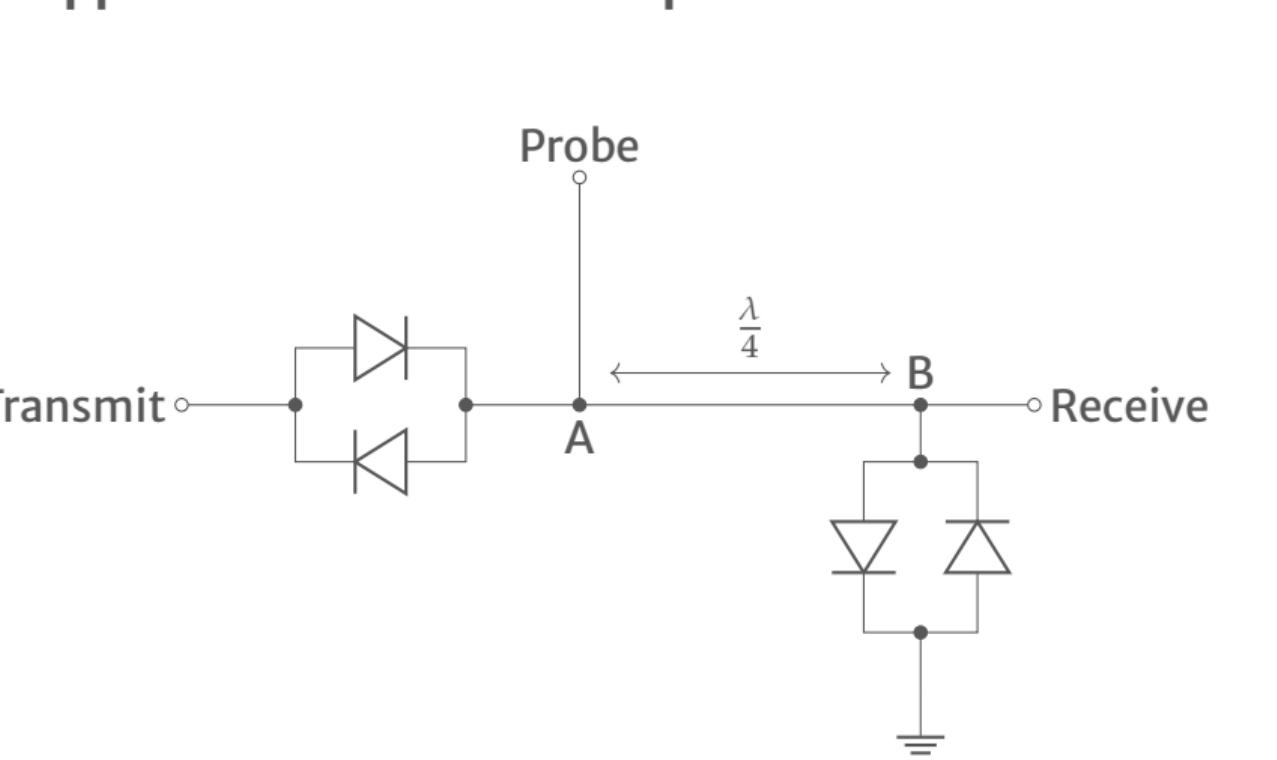
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## └ An amplifier is basically just a transistor

1. We want cheap, so using a simple is the obvious first approach
2. Unfortunately there's a lot to do:
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## The passive approach leaked too much power

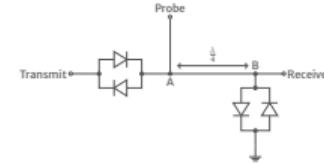


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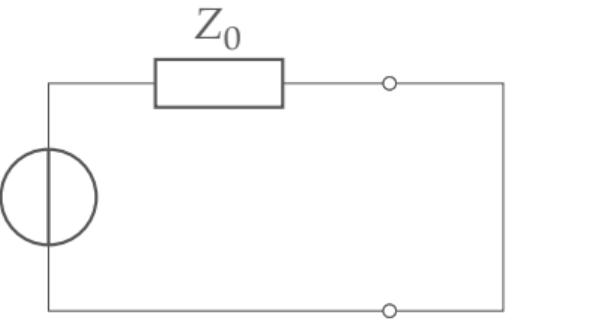
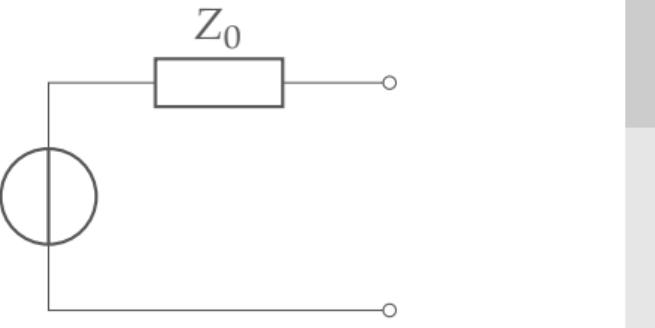
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### └ The passive approach leaked too much power

1. So called "video feedthrough"
2. Especially noise during reception phase, leaking through turned off amplifier
3. "Traditional" passive design by Lowe and Tarr
4. Leads to distortion of low-power pulses
5. Same design can be used with PIN-Diodes (effectively current-controlled resistor)
6. But PIN Diodes often need higher frequencies (mid MHz), size of intrinsic semiconductor



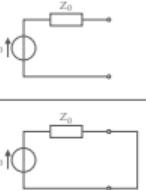
## A transmission line transforms impedance



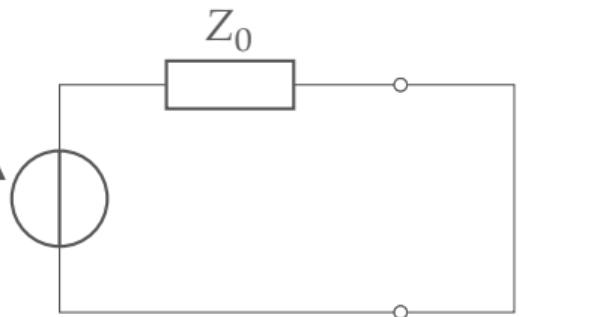
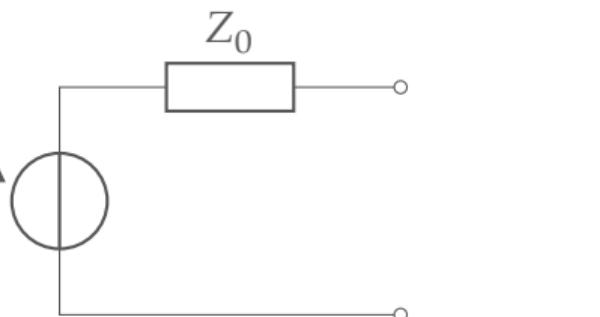
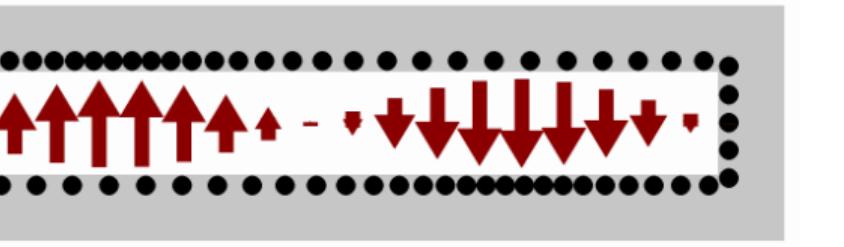
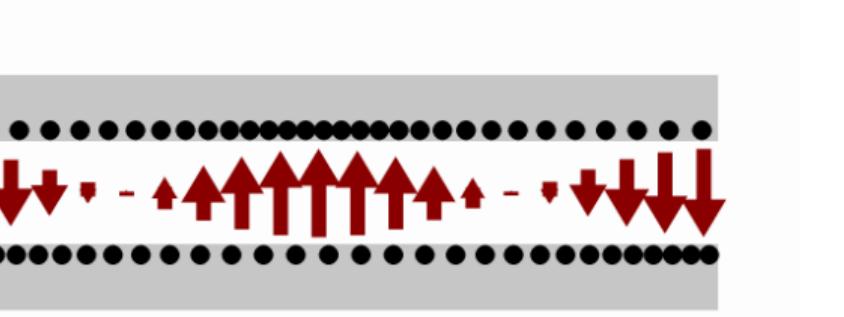
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└ A transmission line transforms impedance



## A transmission line transforms impedance

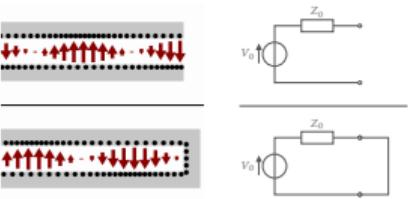


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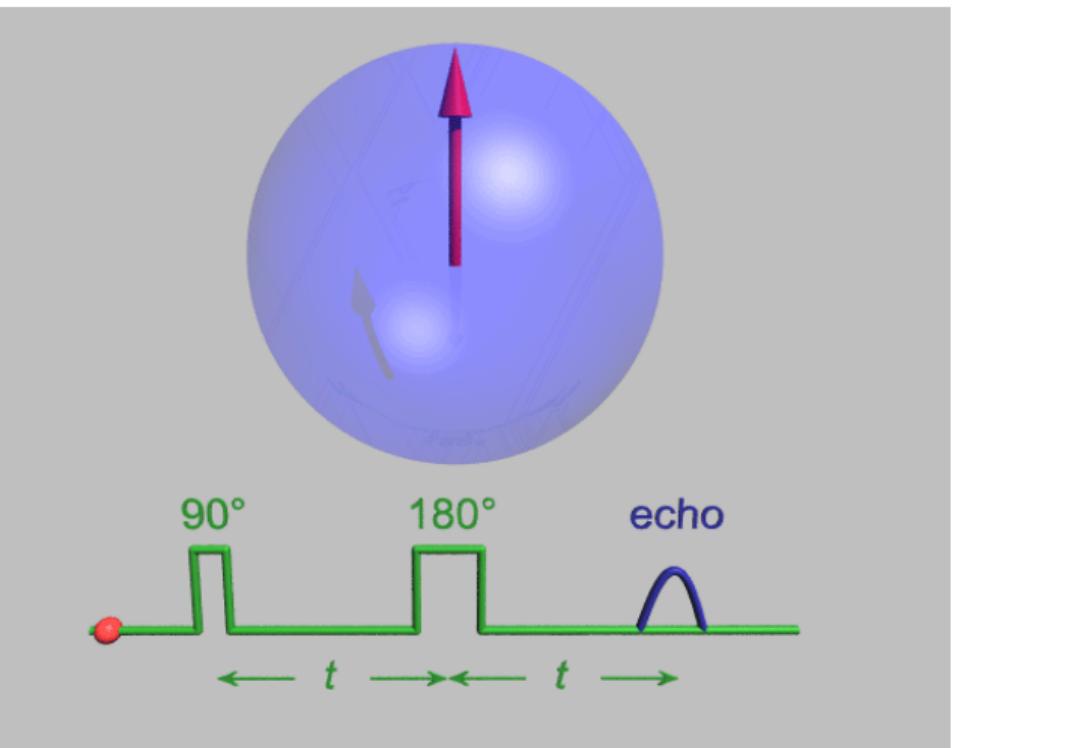
# magnETHical

└ A transmission line transforms impedance

A transmission line transforms impedance



## $T_2$ Decay Animation



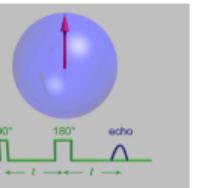
Gavin Morley — CC BY-SA 3.0

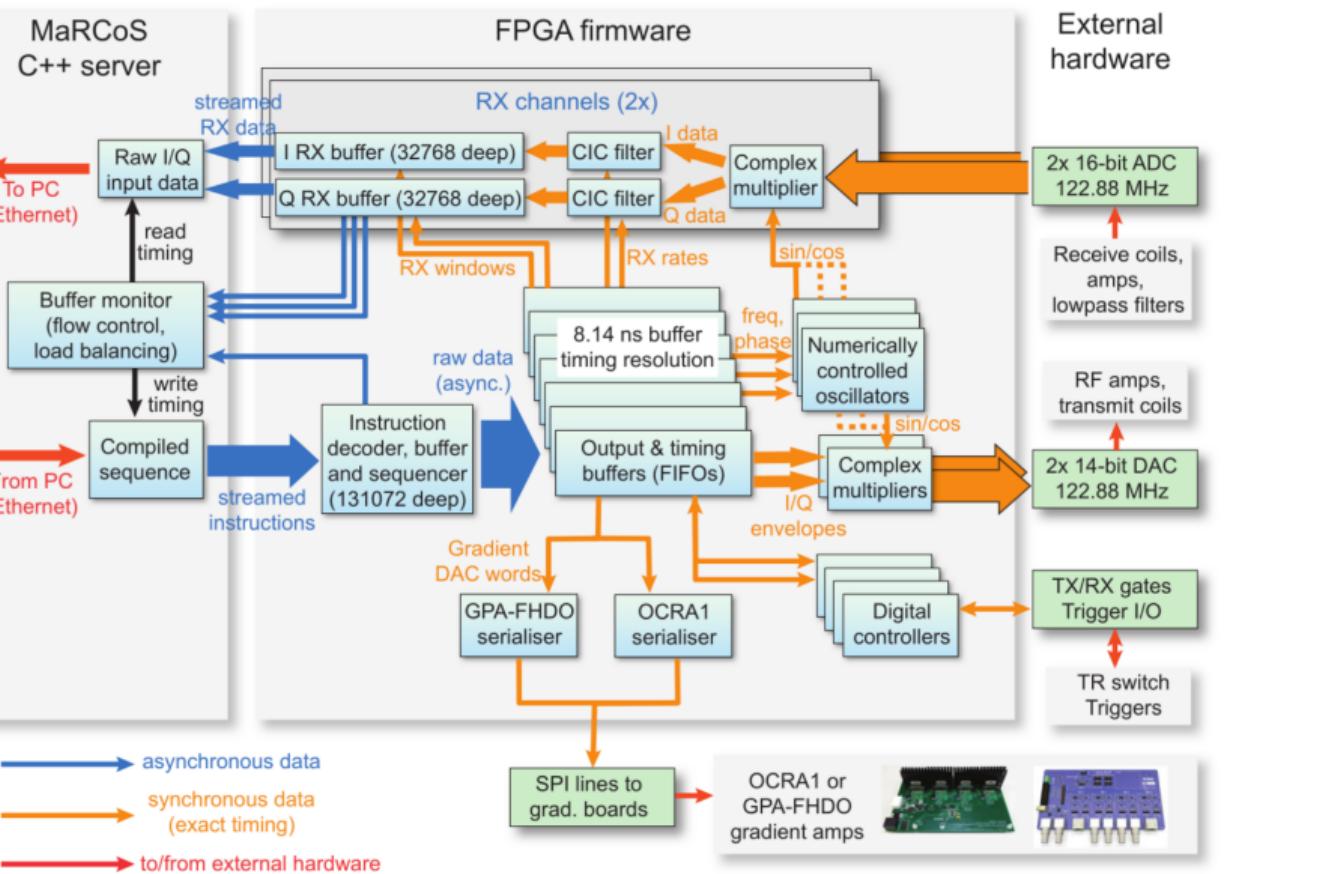
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## $T_2$ Decay Animation

$T_2$  Decay Animation





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└ MaRCoS

