# Non-destructive detection of molecules without mass limitation

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# An experimental and numerical project

The main purpose of this experiment is to develop an original detector for mass spectrometry.

GiantMol prototype

- Molecular source
- $Ca^+$ trap
- Laser cooling

Numerical simulations

- GMol $\rightarrow$ $Ca^+$ interaction
- Molecular ion guiding through 80cm

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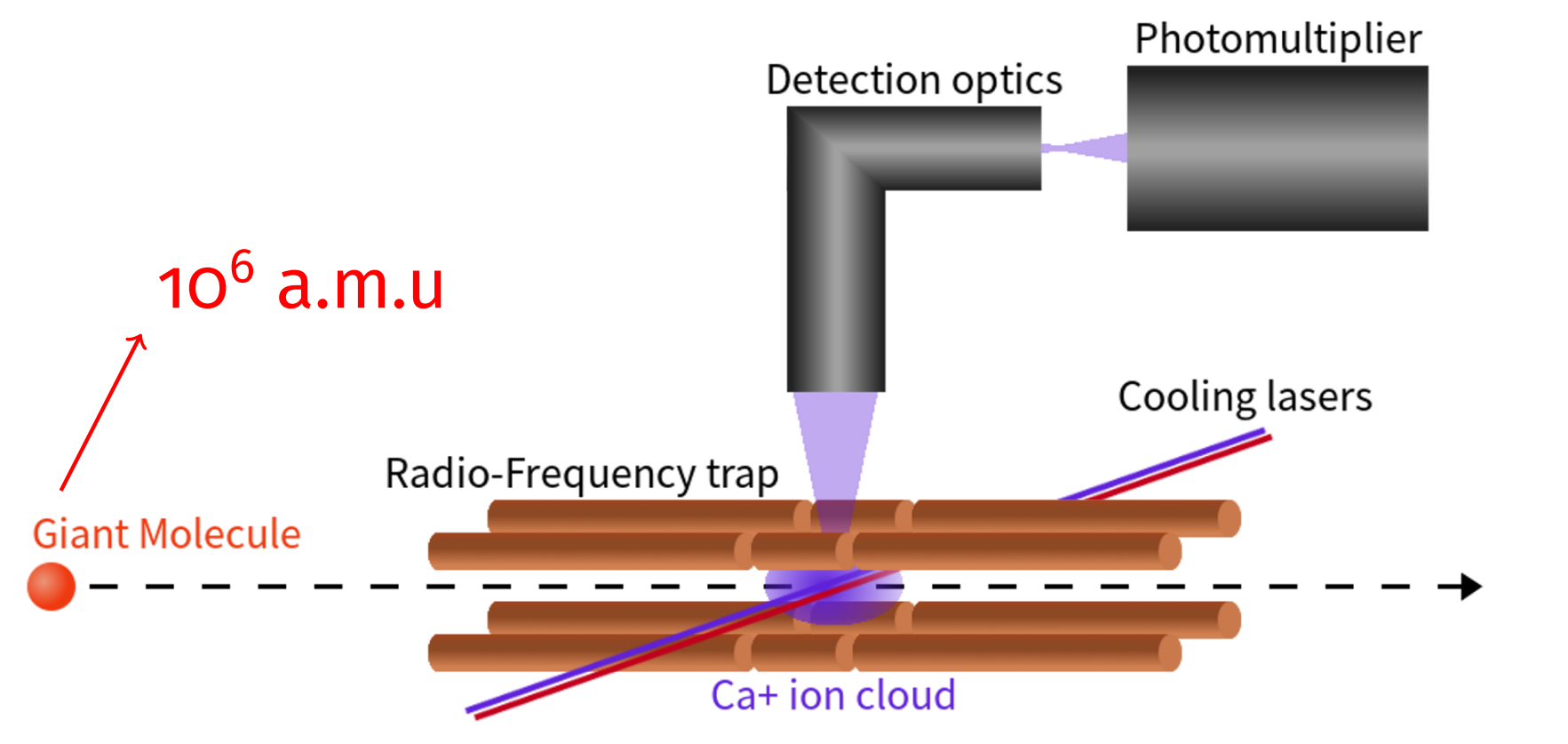
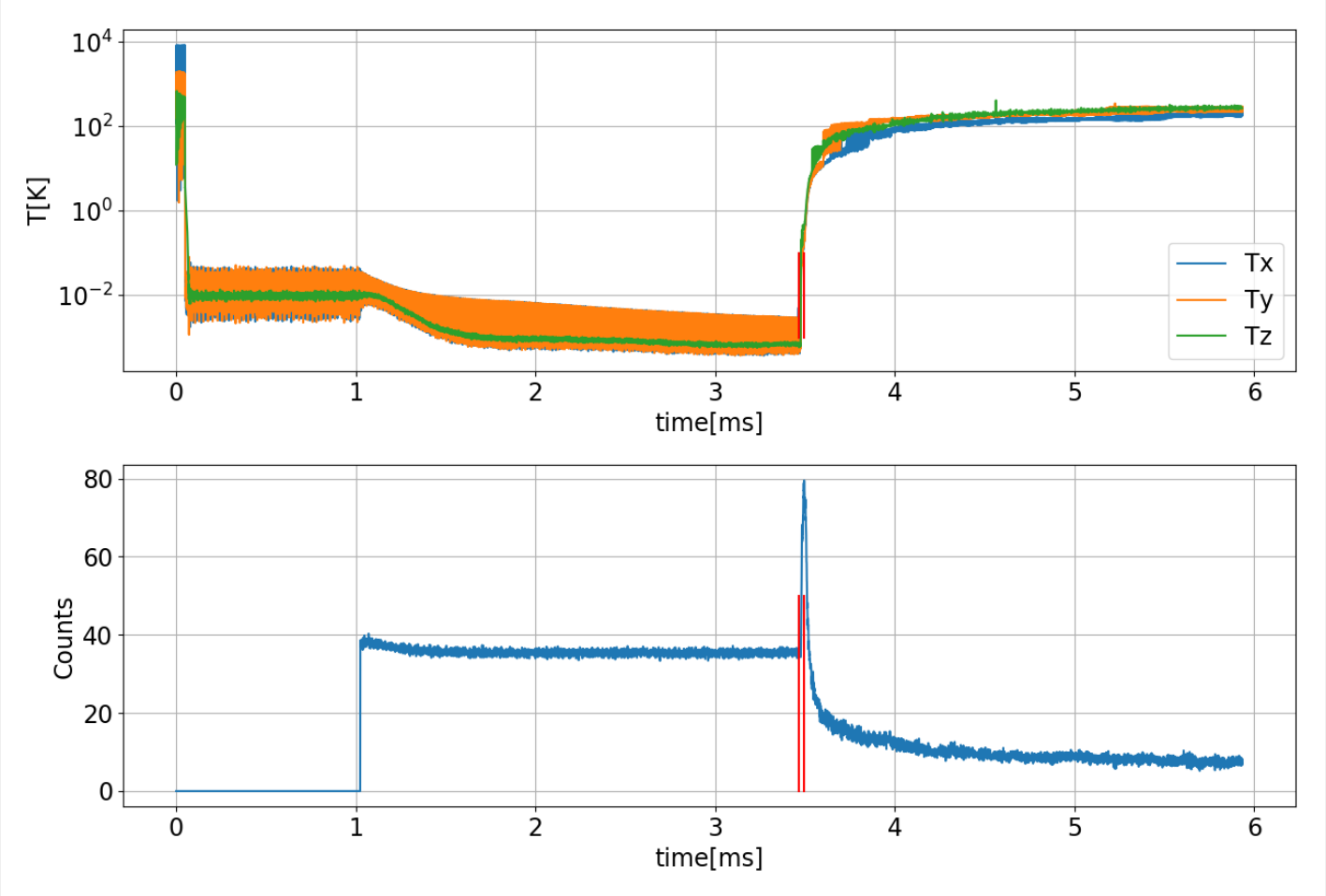
# Principle of the experiment




The Giant Molecule crossing the ion cloud produces a perturbation which modifies the fluorescence.

# Principle of the experiment

Ion temperature and fluorescence during a simulated interaction.



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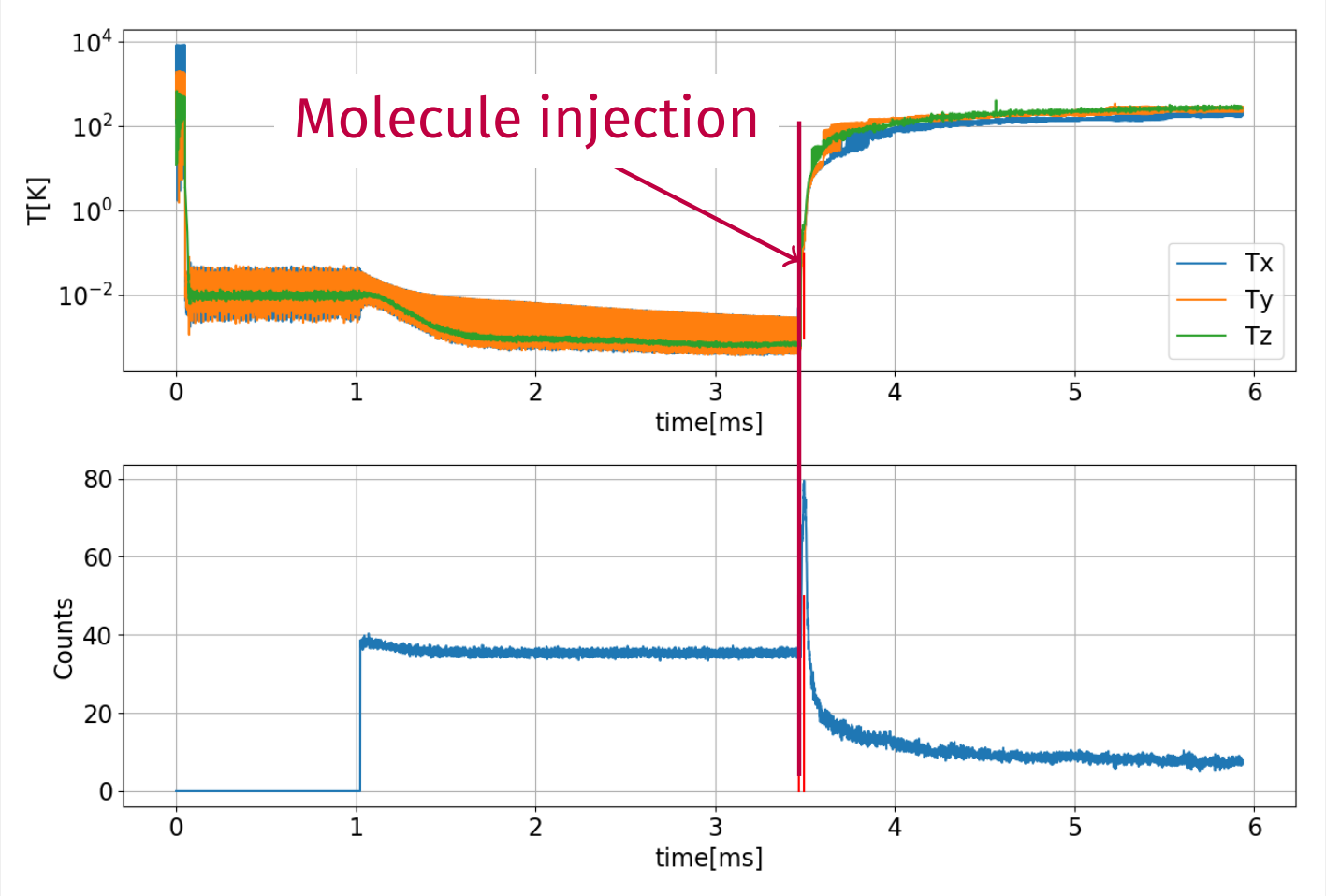
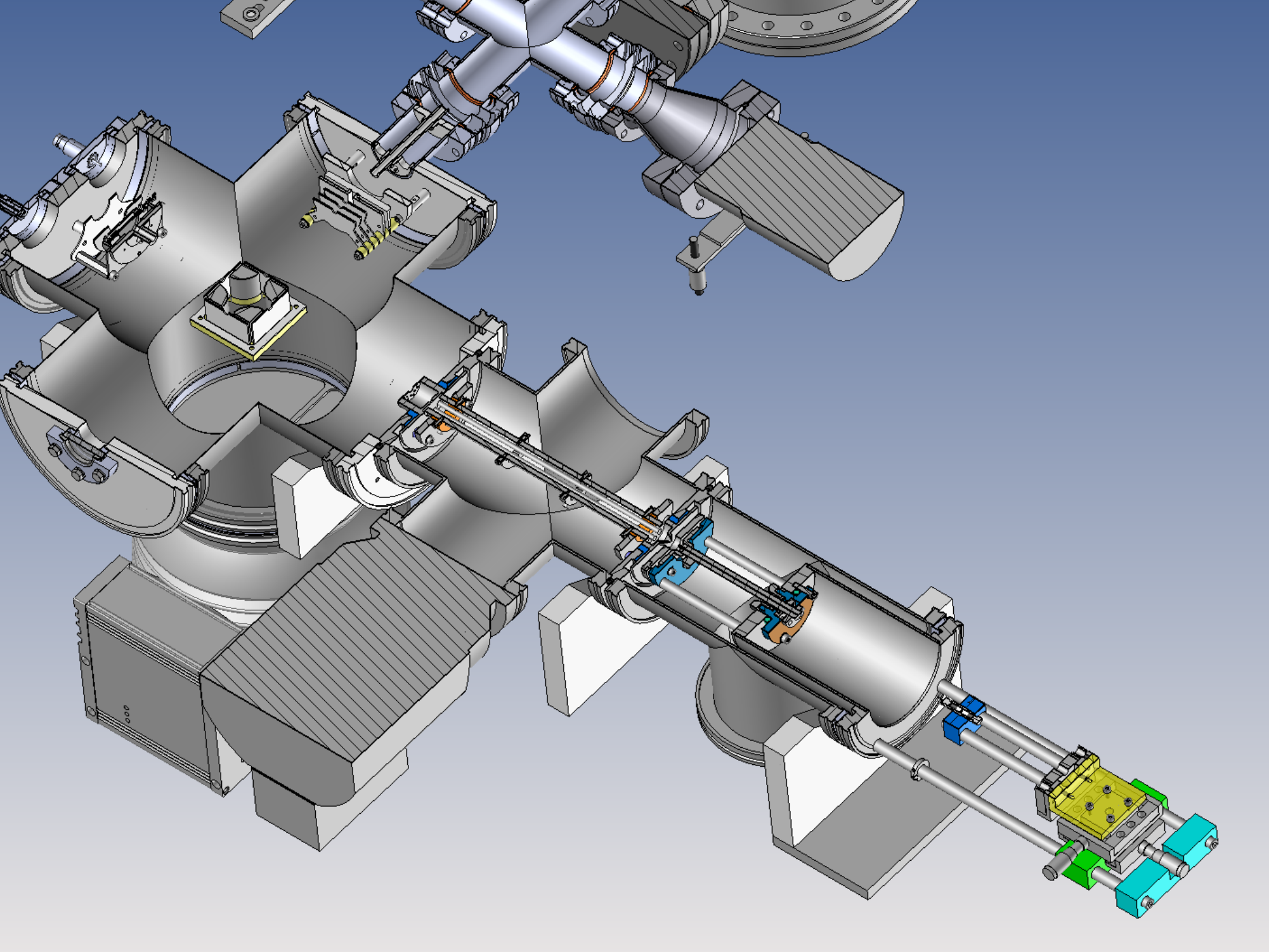
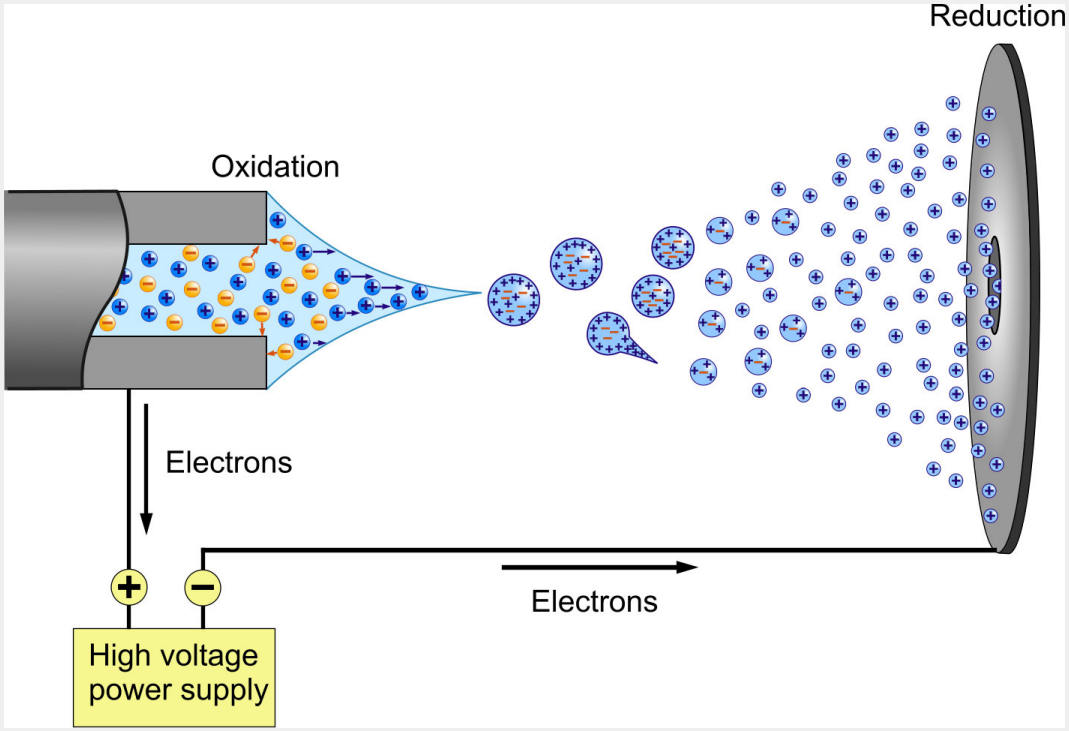


# Experimental setup



# Molecular source - Electrospray




Electrospray source positive mode (CC Andreas Dahlin)

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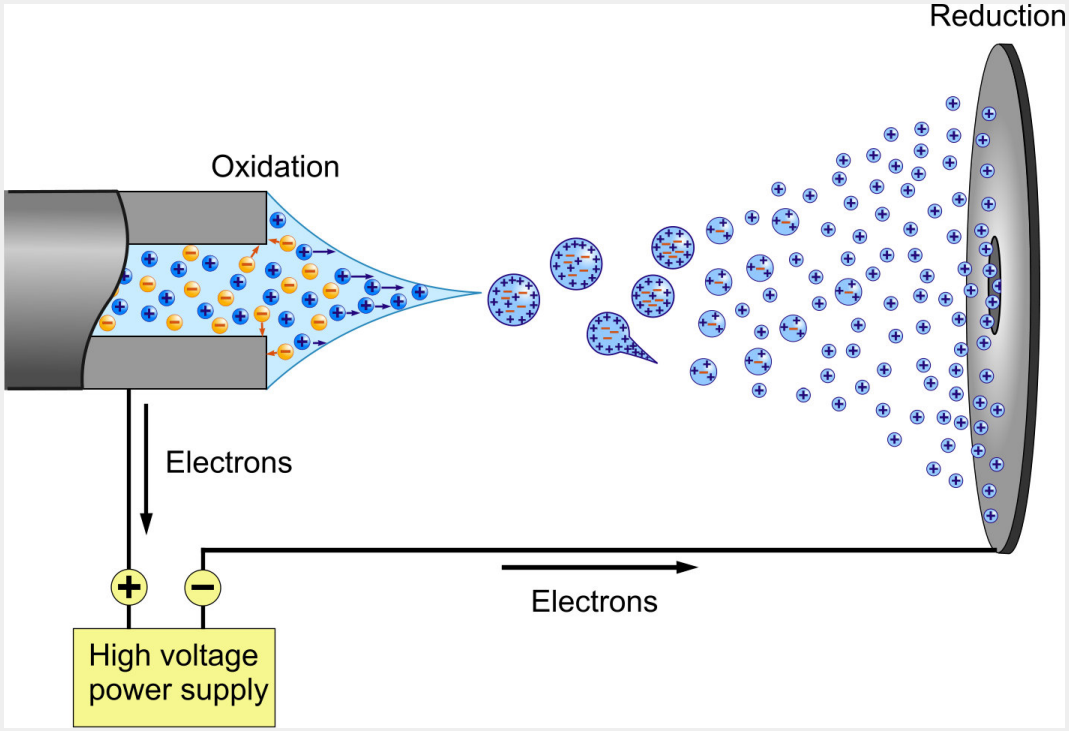


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Rayleigh stability condition

$$Q^2 = 16\pi a_0^3 \sigma$$

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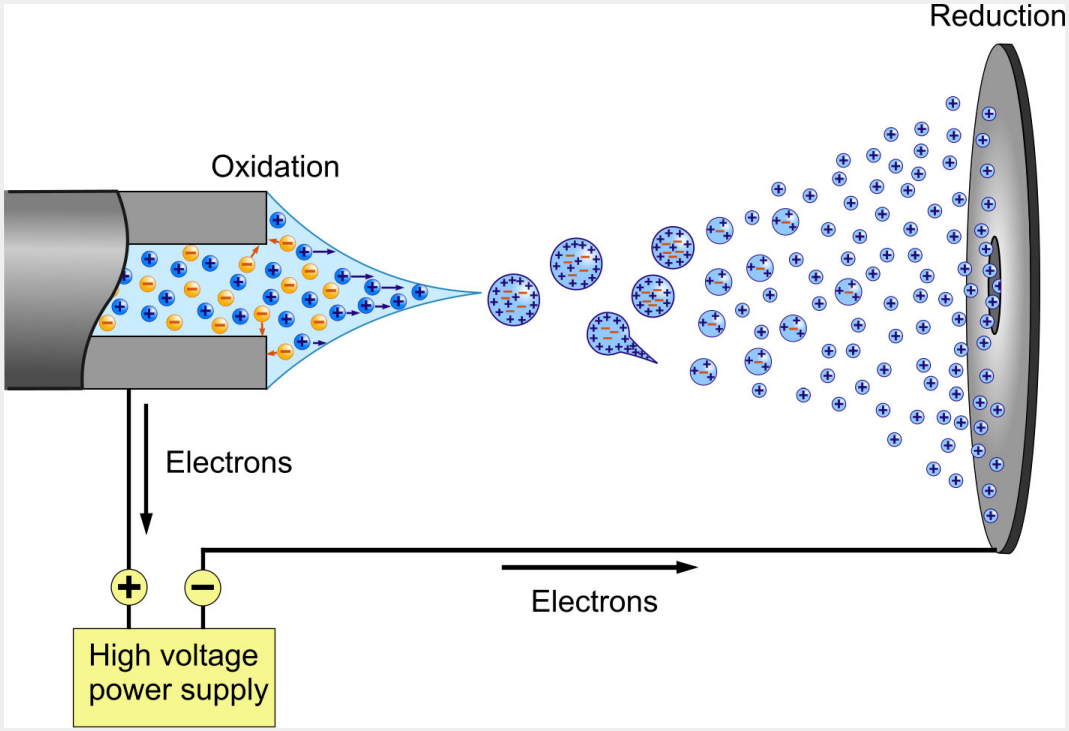


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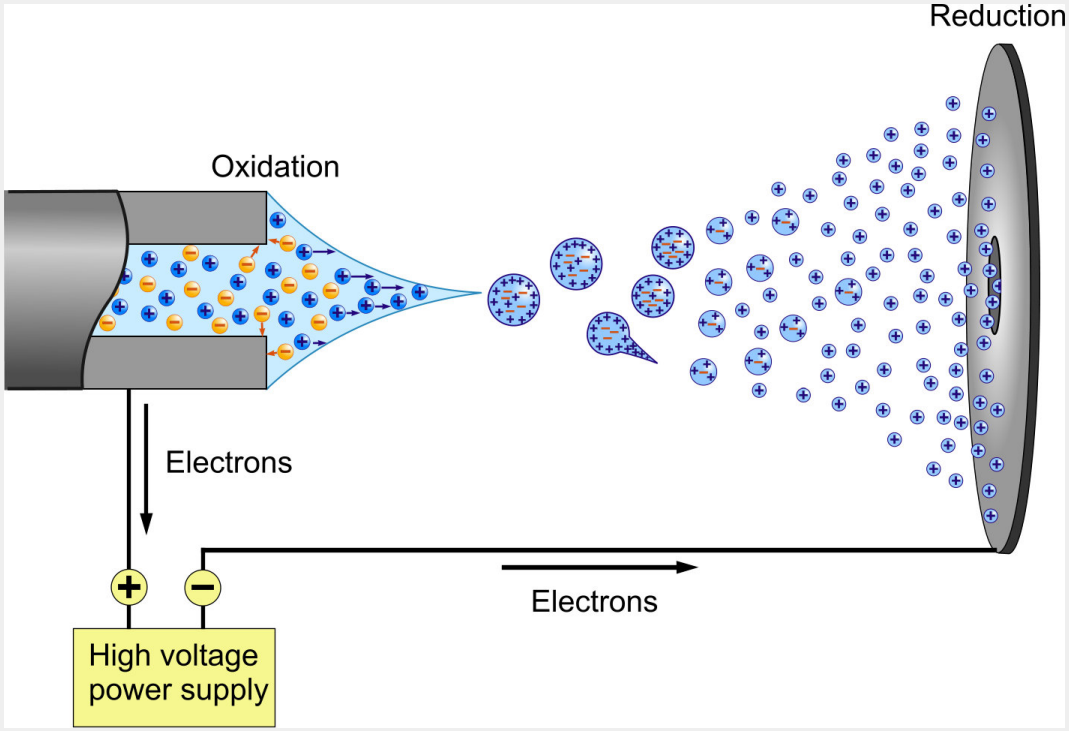


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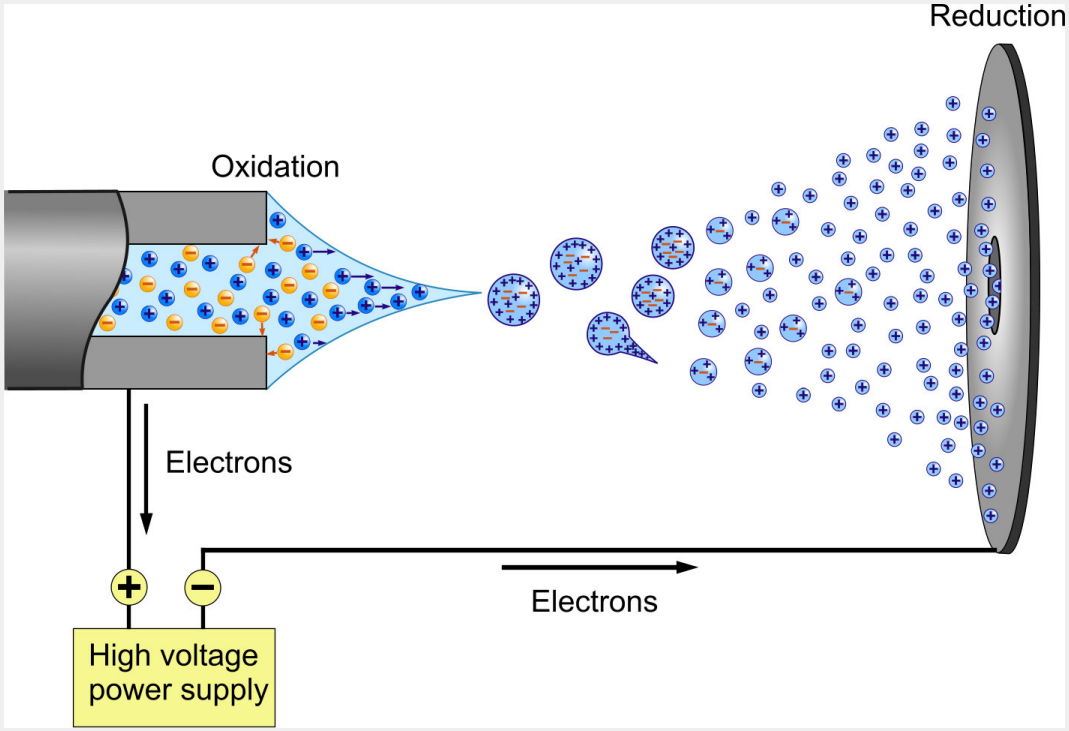


Electrospray source positive mode (CC Andreas Dahlin)

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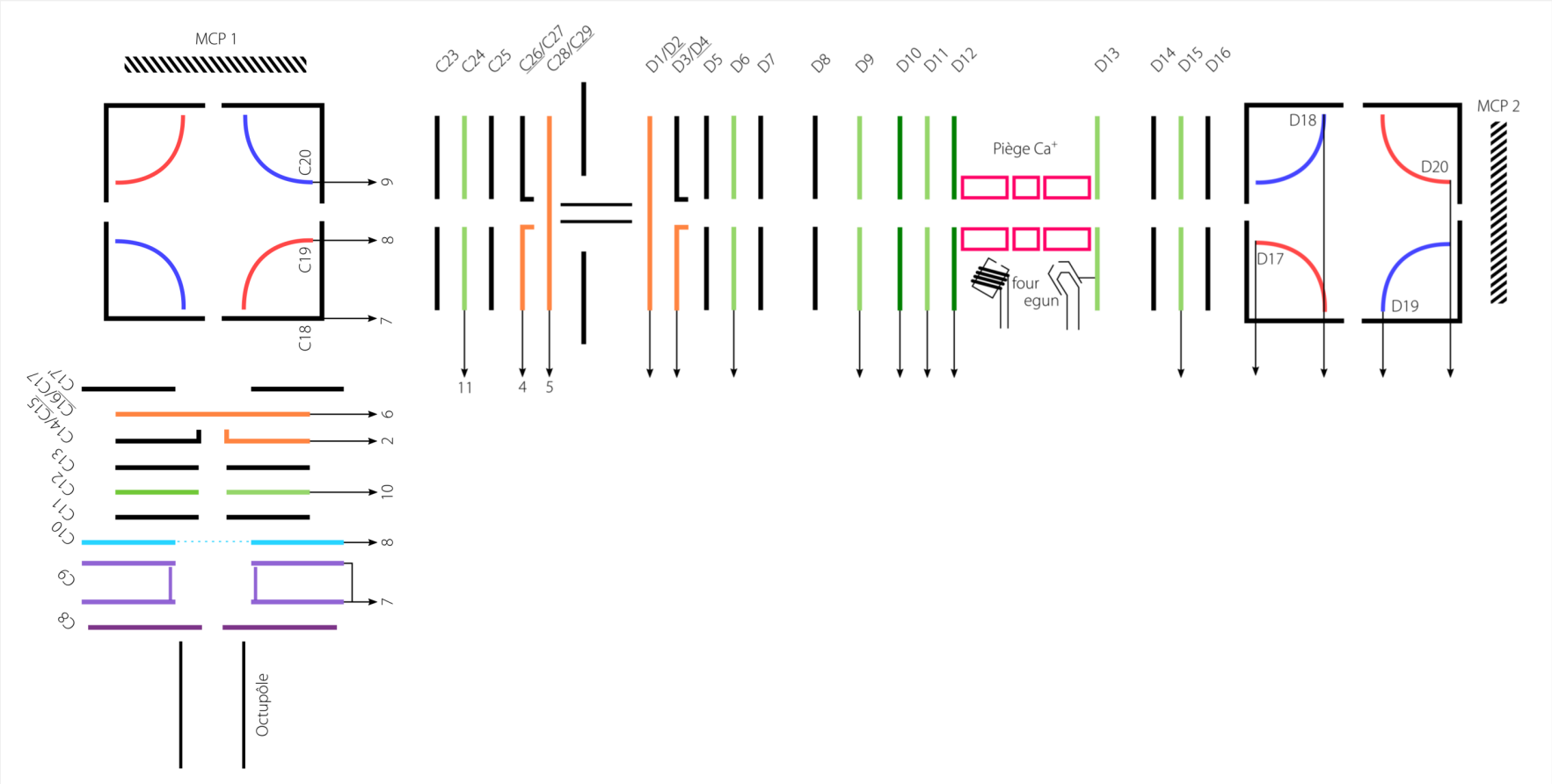
charge

surface tension

$$V = \frac{Q}{a_o}$$
$$= \sqrt{16\pi a_o \sigma}\ (\text{cgs})$$

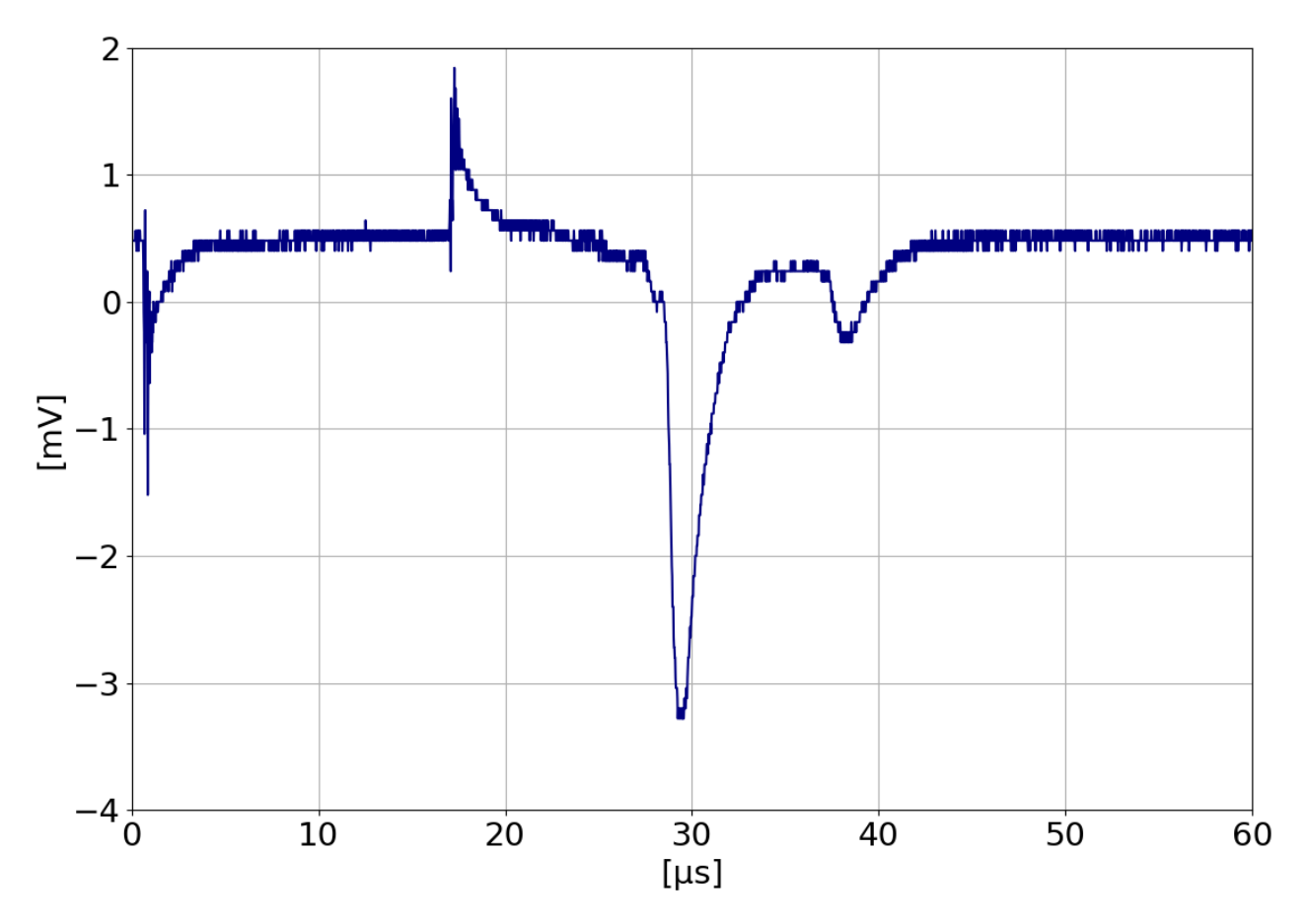
For a 1mm water droplet $V \approx 6000V$

# Molecular source - Electrospray




Electrode layout from octupole to MCP's.

# Molecular ion detection halfway



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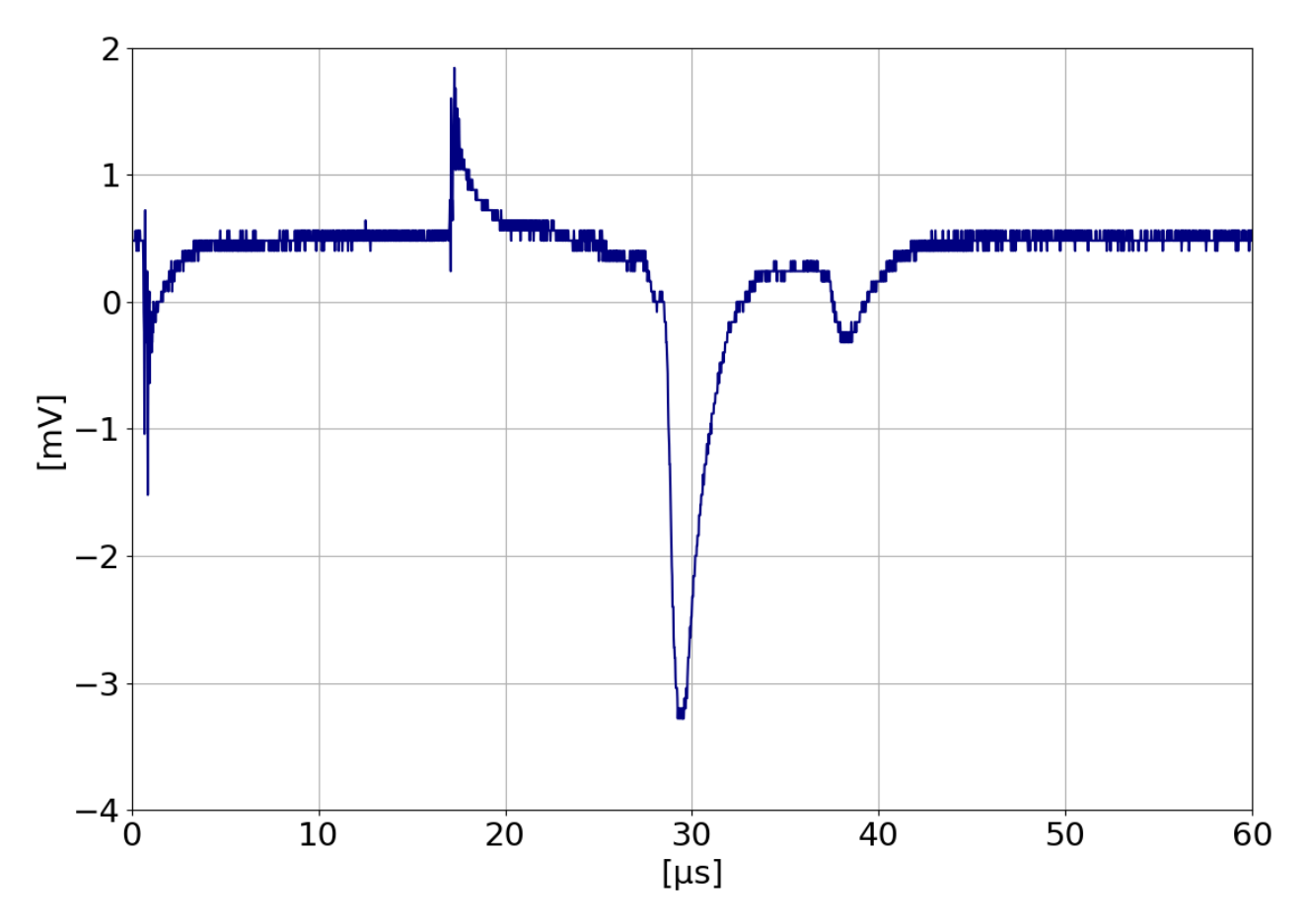
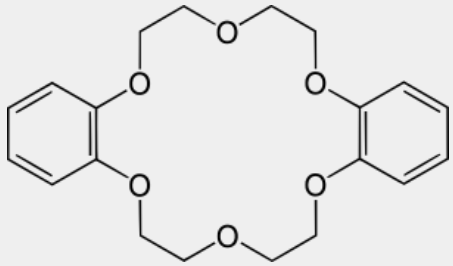
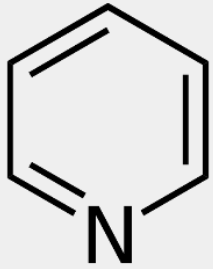



DiBenzoCrown Ether 360 a.m.u.




Pyridine 79 a.m.u.

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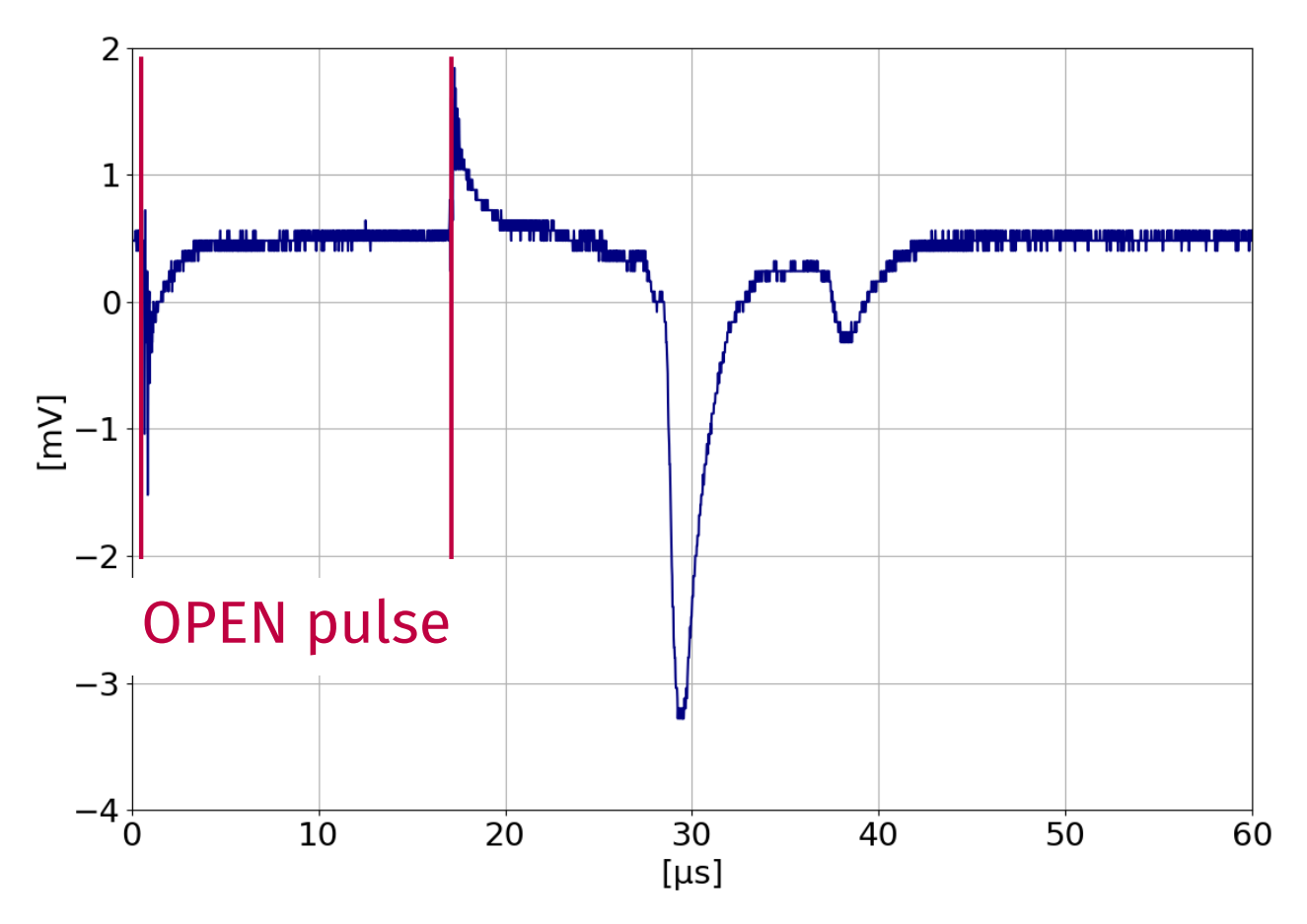


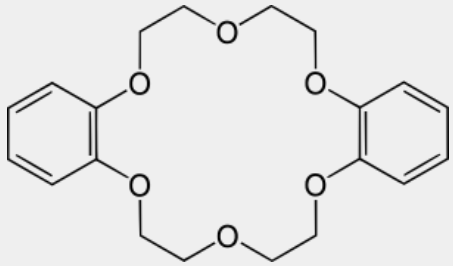

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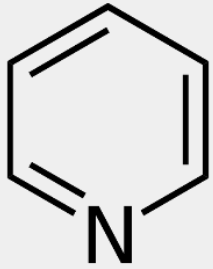


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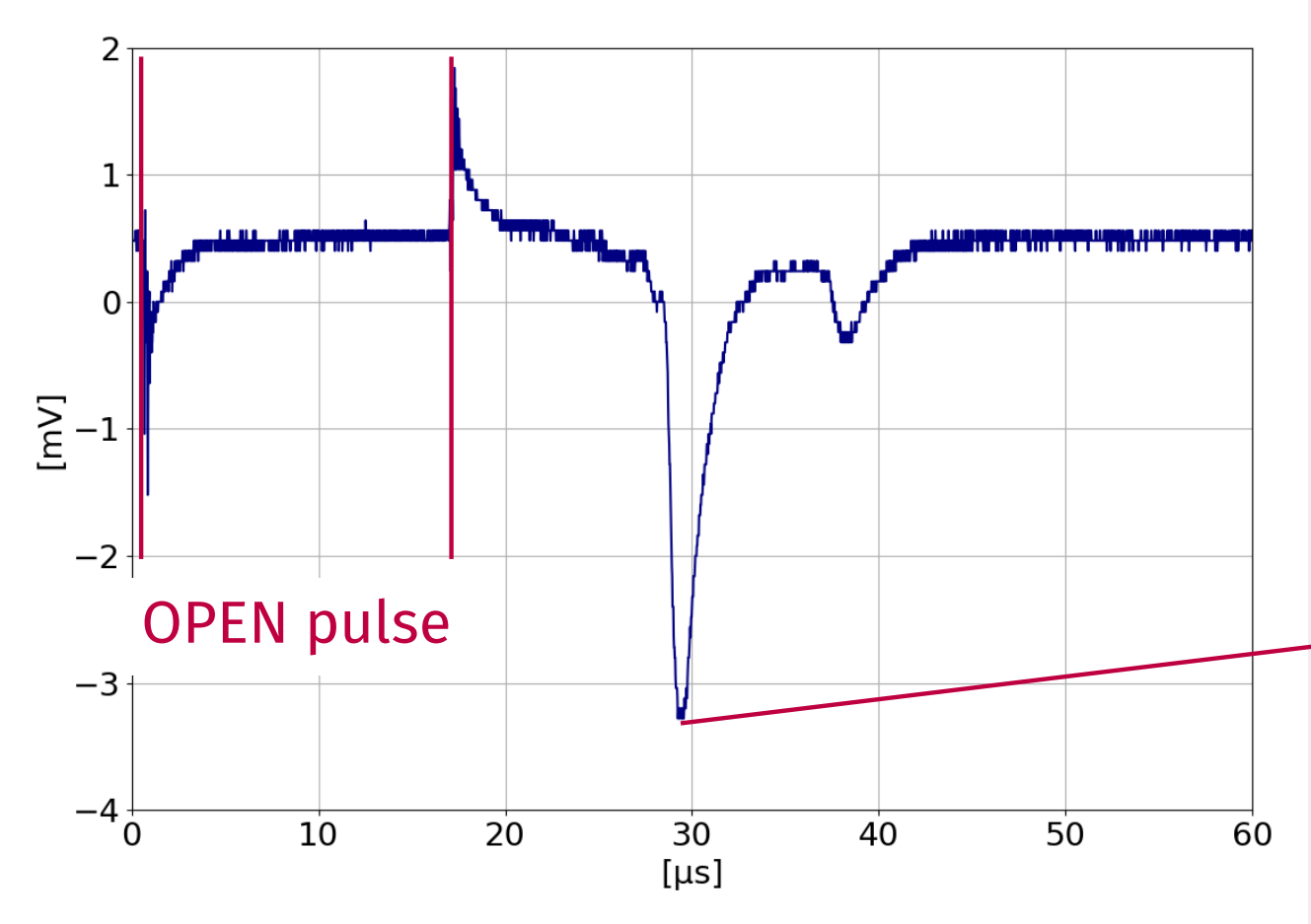


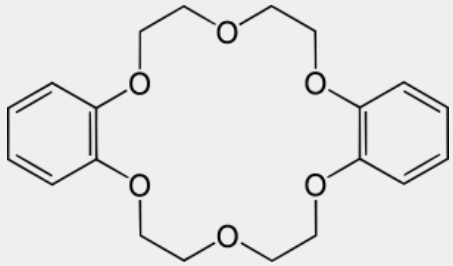

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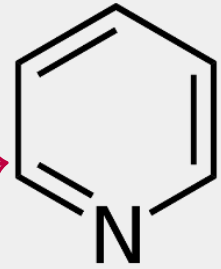


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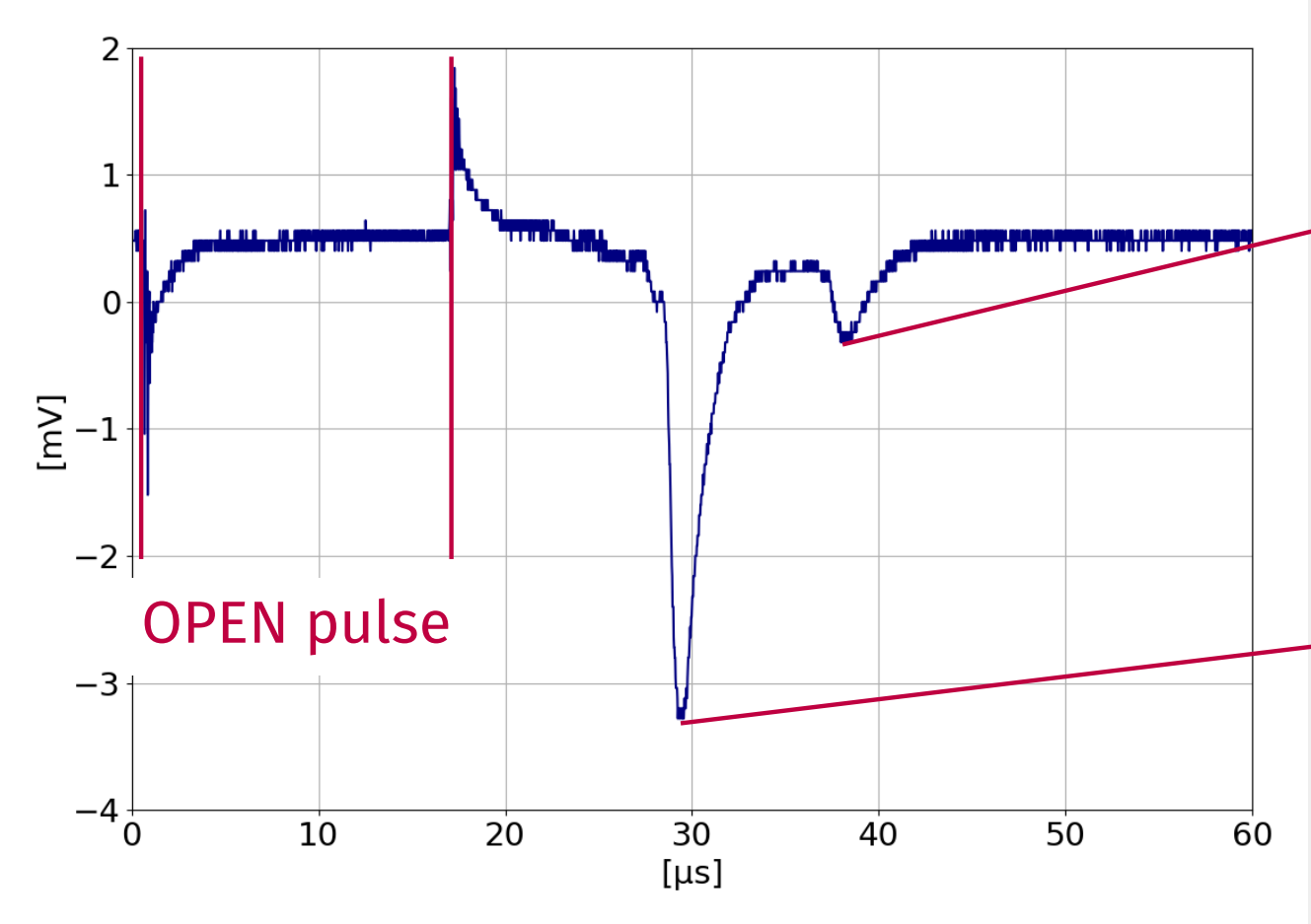


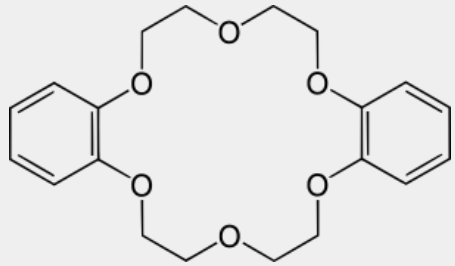

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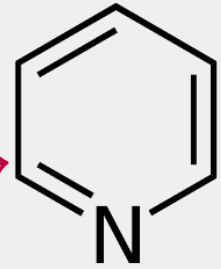


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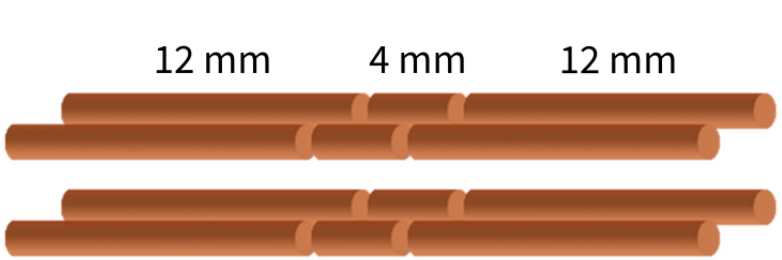
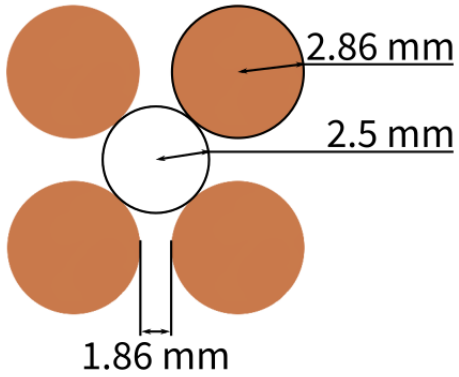
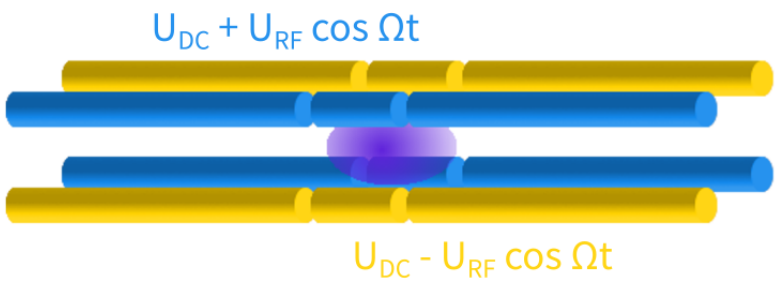
# Molecular ion detection after the trap

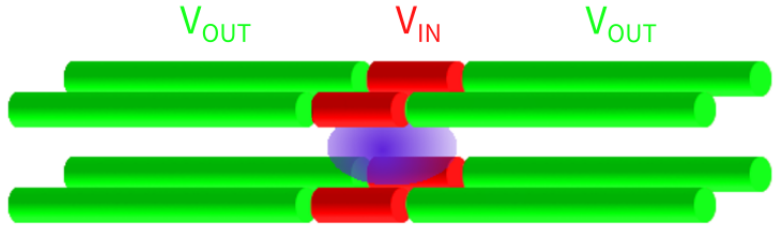
Molecular ion count with MCP after the trap. 20 samples mean.

# Ion trapping




Size and power supply for the quadrupolar trap.

Potential between two rods

$$\Phi_r(x, y, t) = (V_{DC} + V_{RF}\cos(\Omega_{RF}t))$$

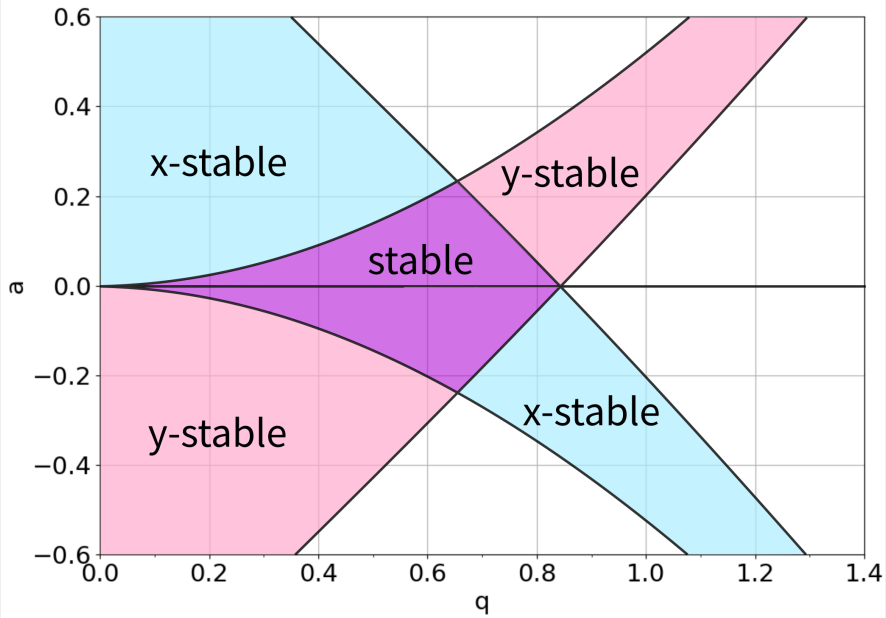
Motion equation (single ion)

$$0 = \ddot{u} + (a_u - 2q_u\cos 2\tau)u$$

with $u = x, y$ and $\tau = \dfrac{\Omega_{RF}t}{2}$

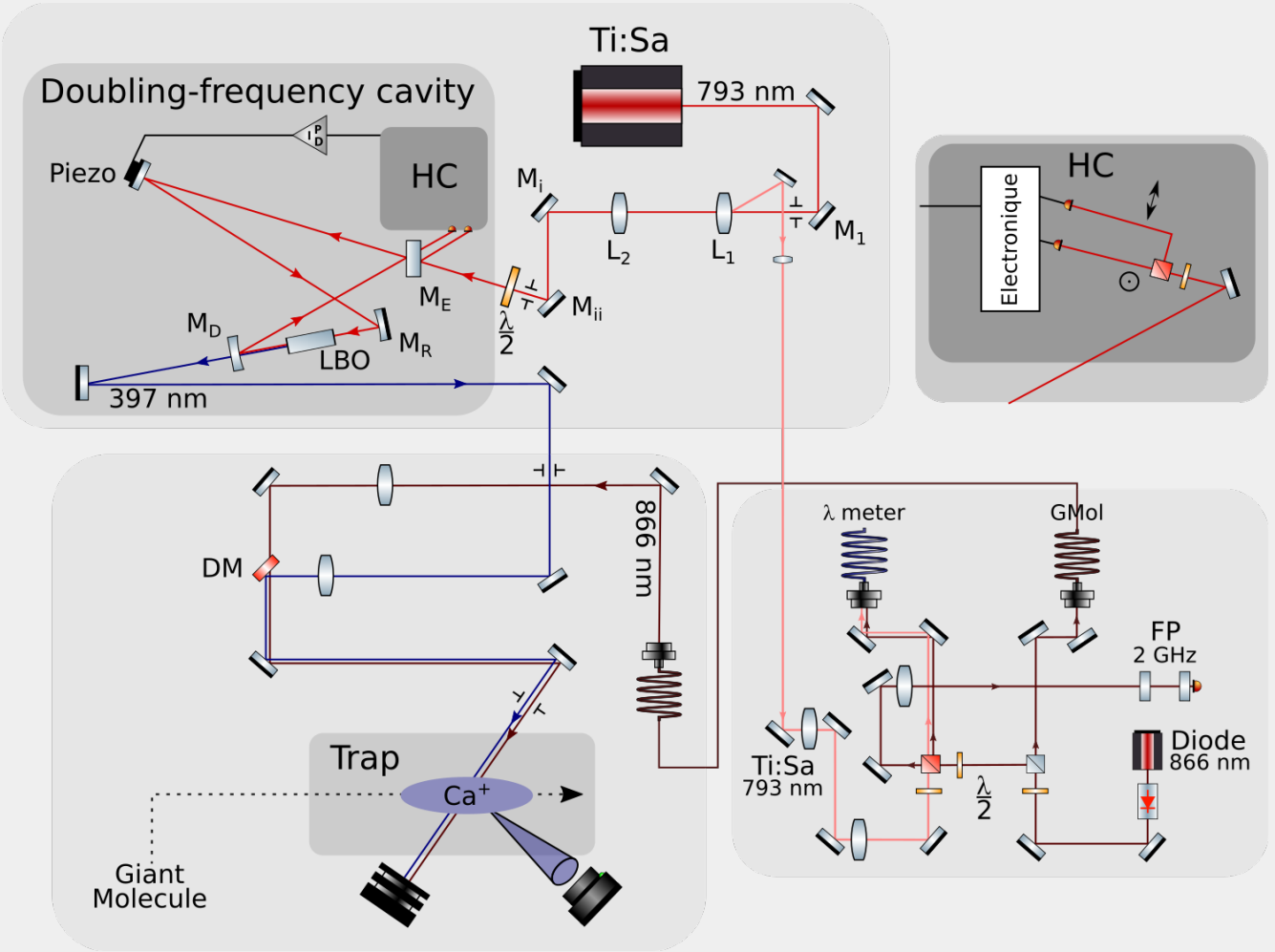
$$a_x = -a_y = \frac{4eU_{DC}}{mr_0^2\Omega_{RF}^2}$$

$$\text{and } q_x = -q_y = \frac{2eU_{RF}}{mr_0^2\Omega_{RF}^2}$$

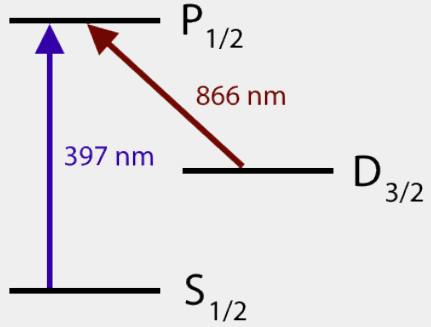



Stability diagram for the quadrupolar linear trap.

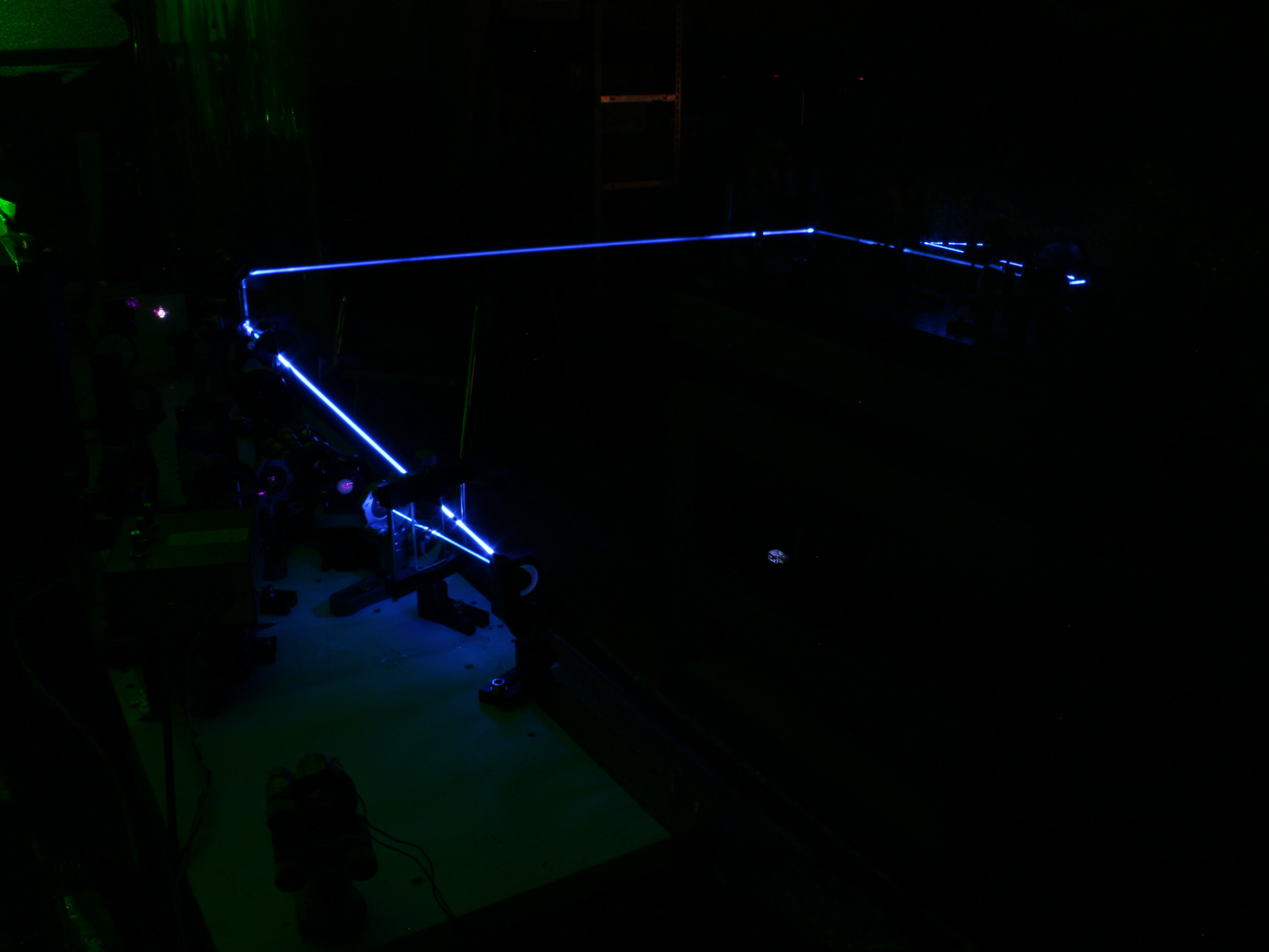
# Laser cooling



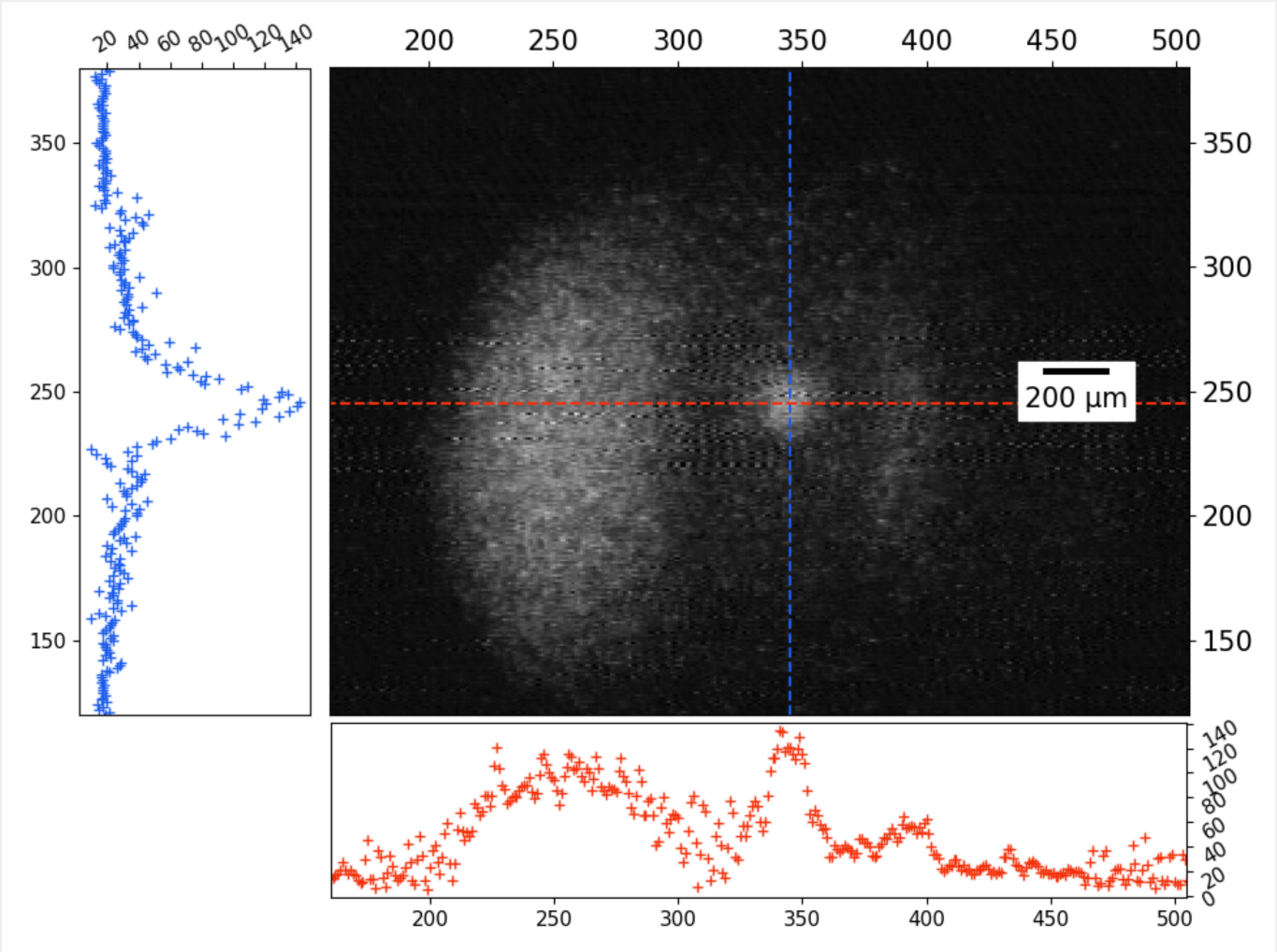

Laser cooling setup.




$Ca^+$ energy levels.

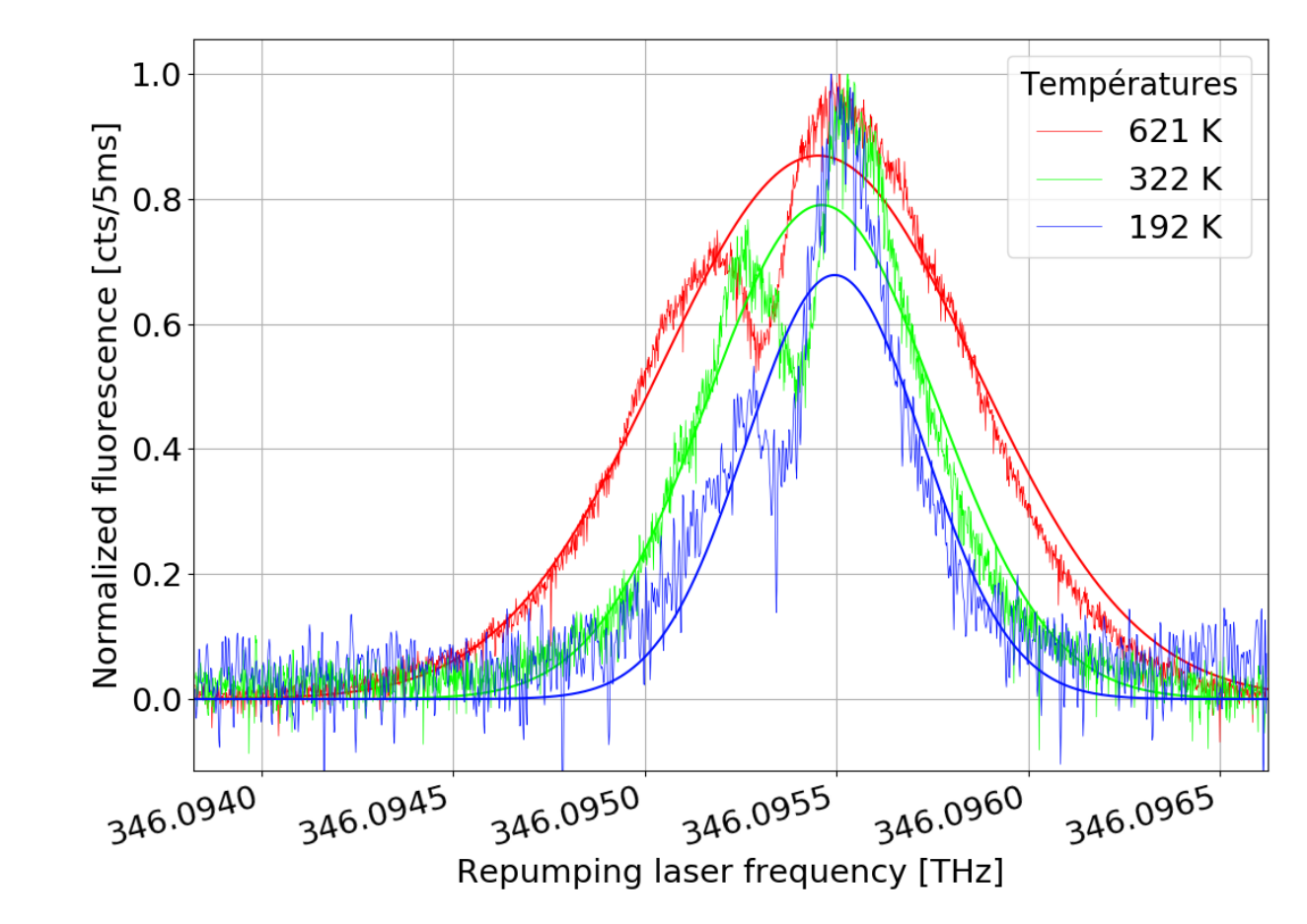


# $Ca^+$ cloud profile




Ion cloud with profile and scalebar.

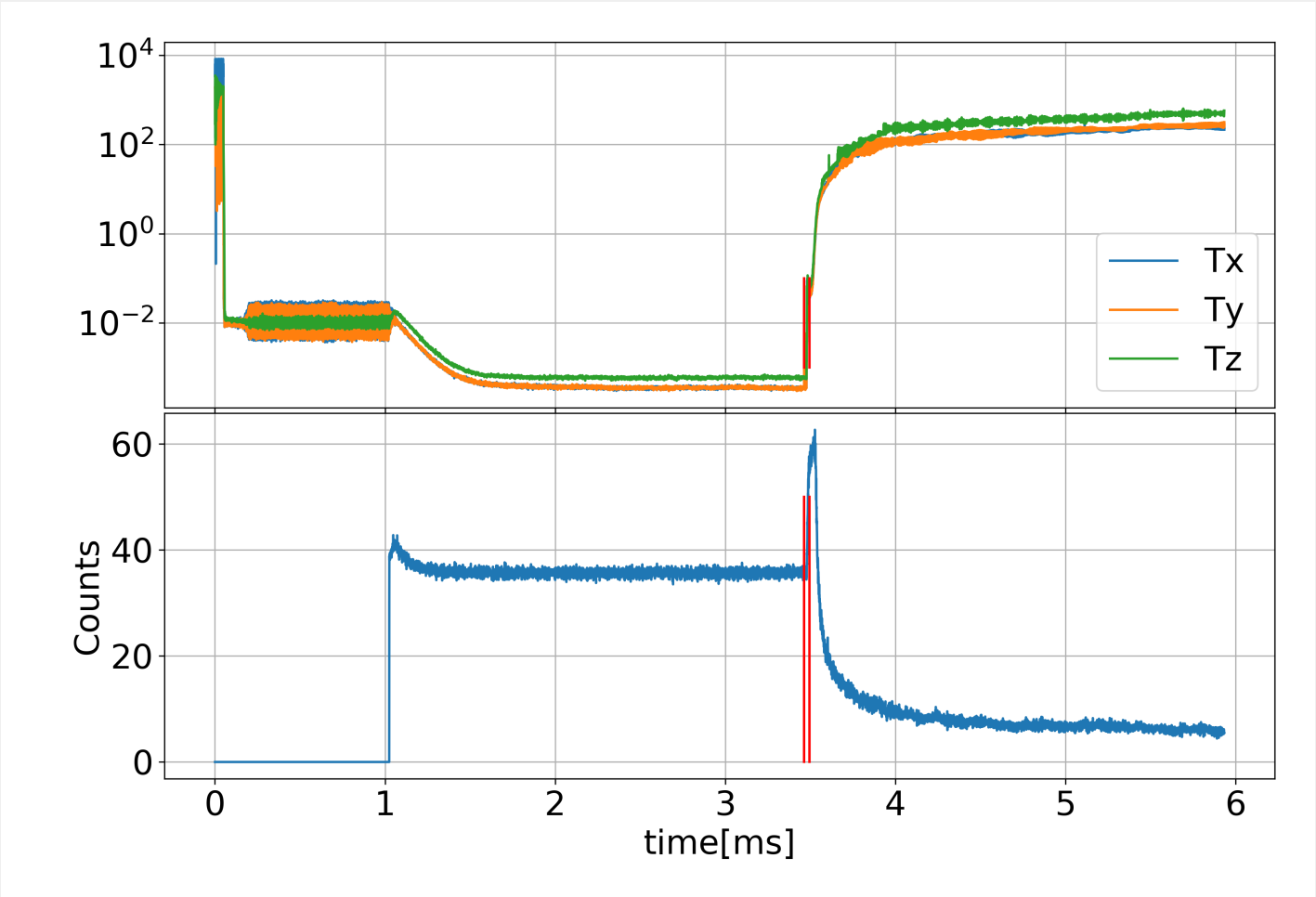
# $Ca^+$ cloud temperature




Three different fluorescence profiles for three red laser scans.
Narrower the curve, colder the cloud.

# GMol → $Ca^{+}$
# INTERACTION SIMULATION

# Detection signal




Detection signal as a *significant* fluorescence evolution.

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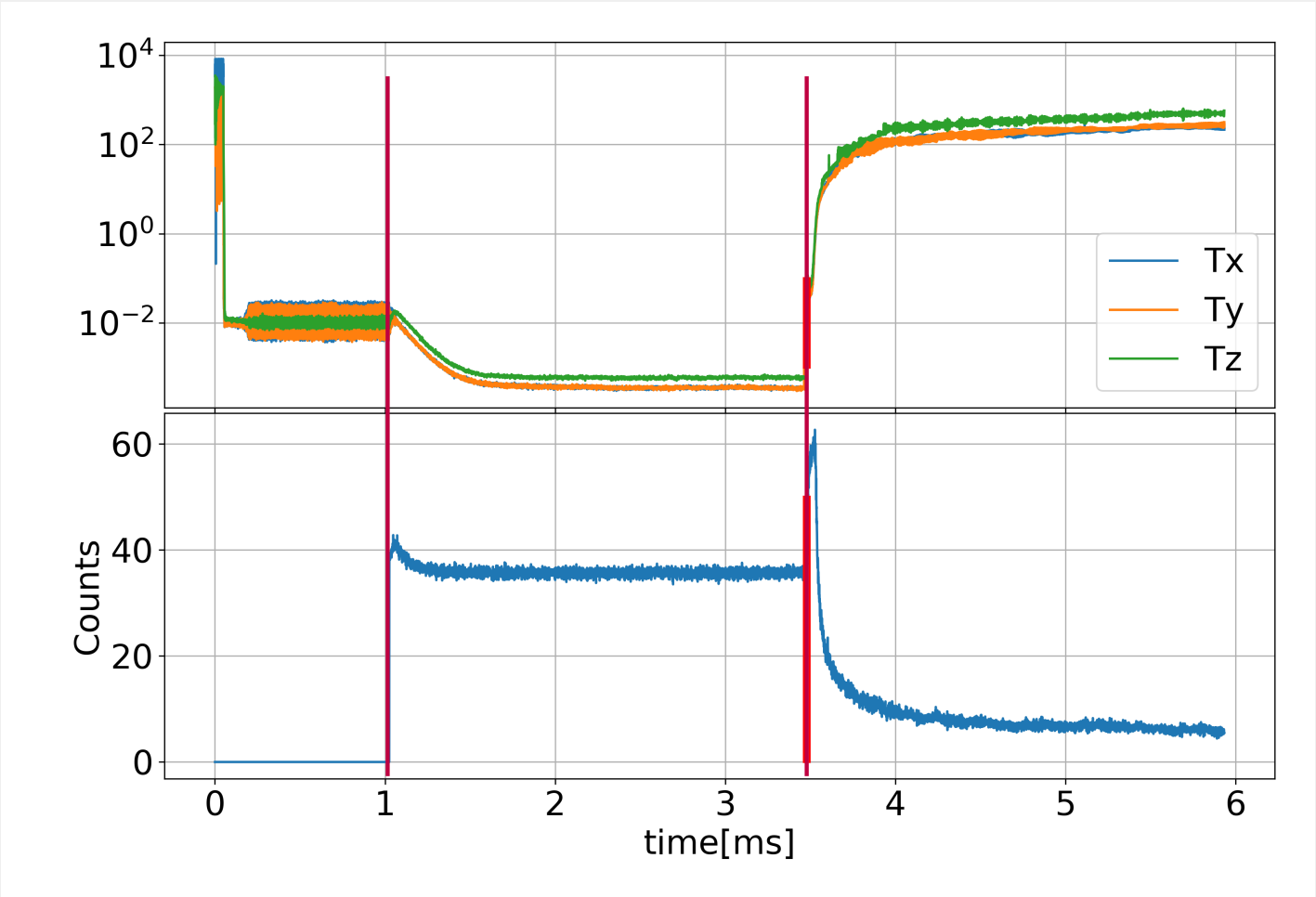


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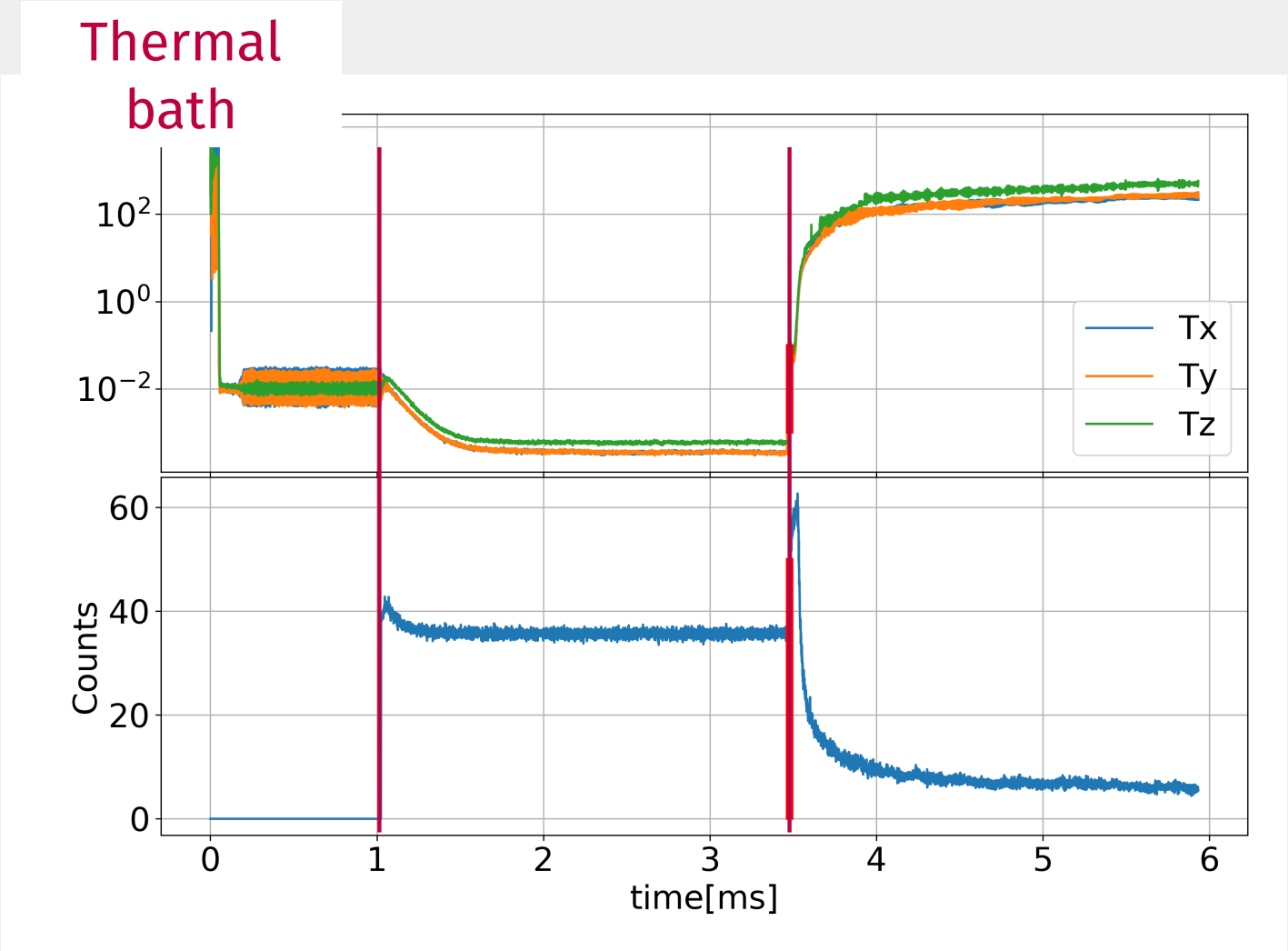


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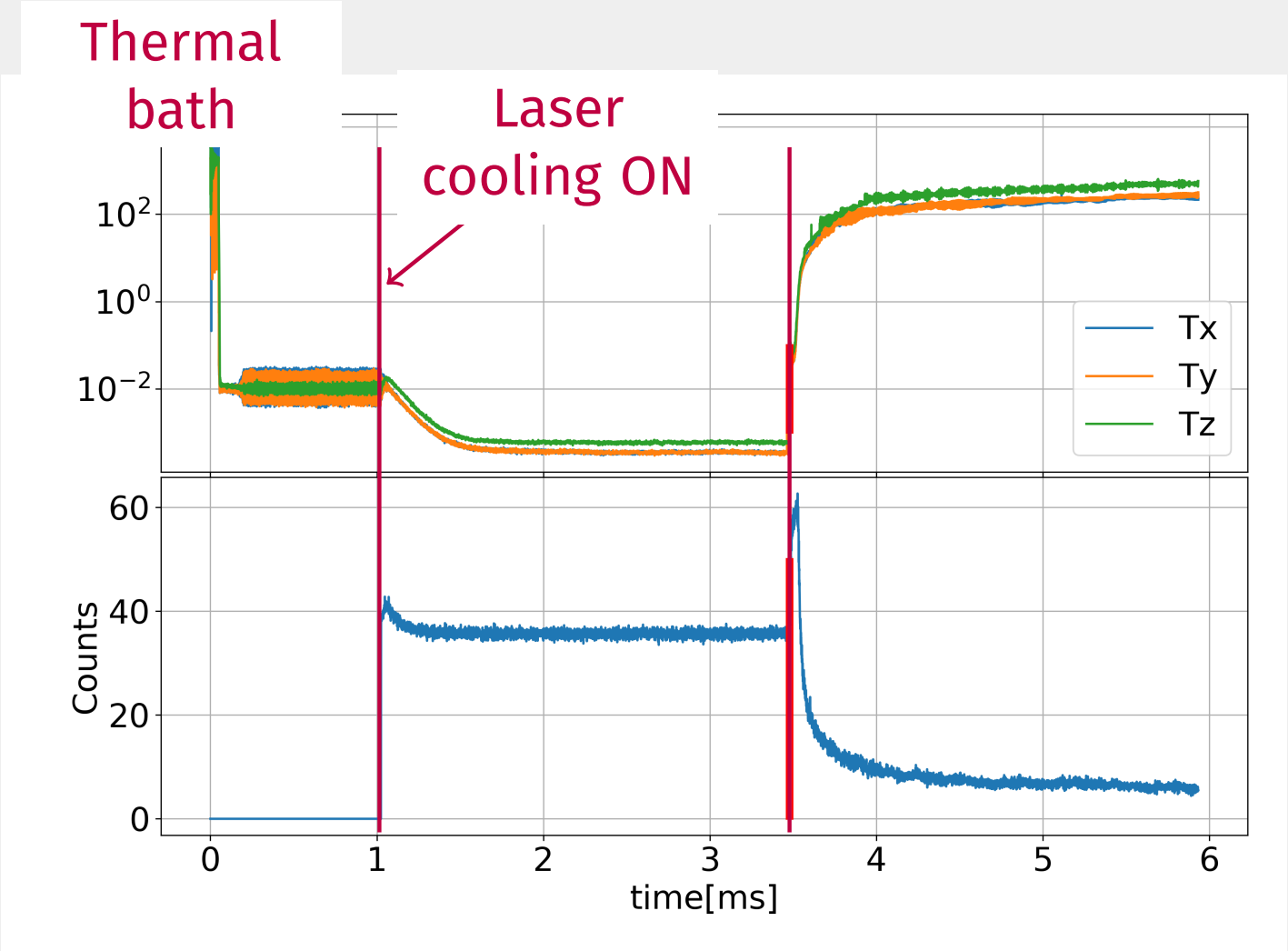


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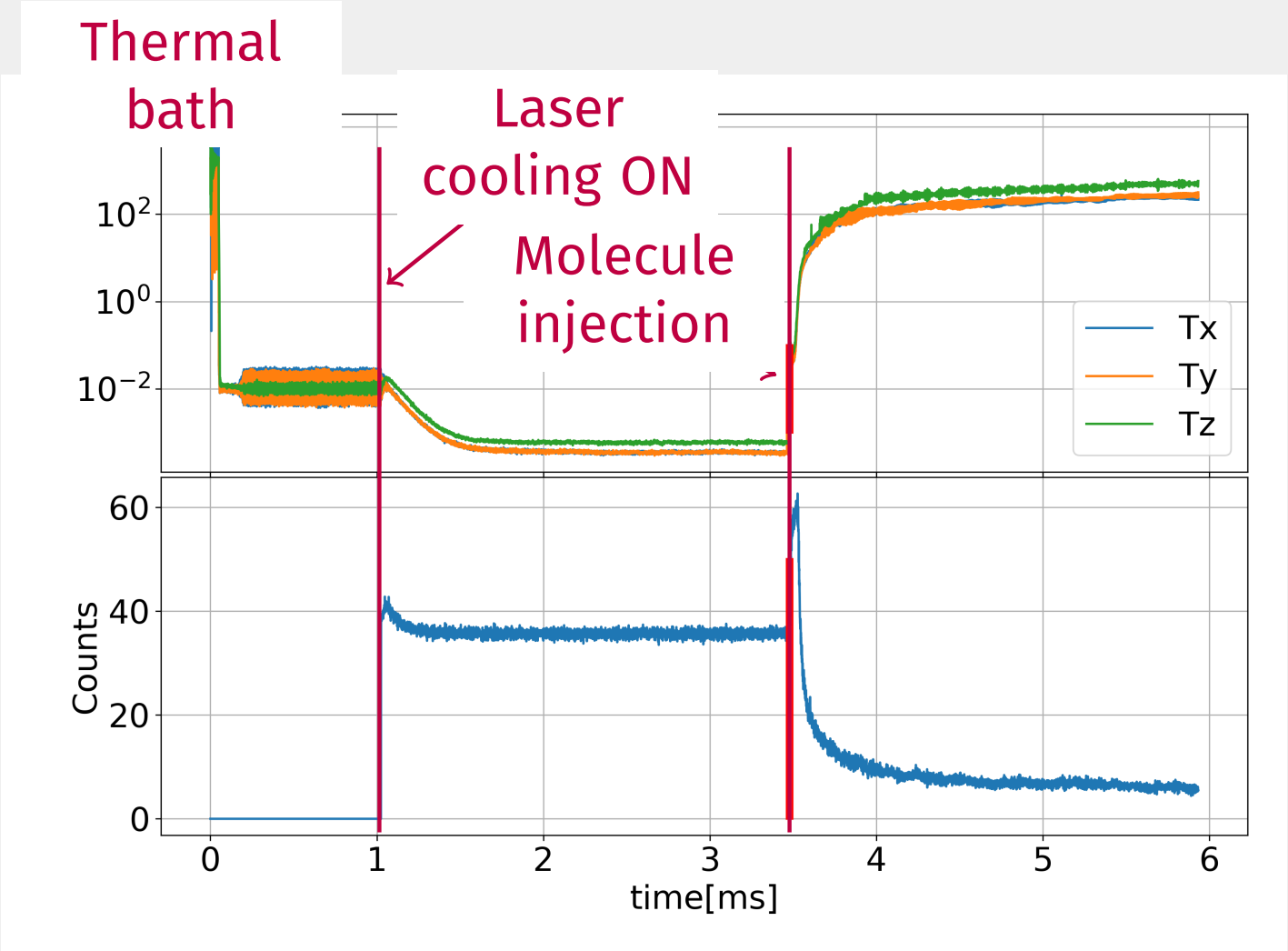


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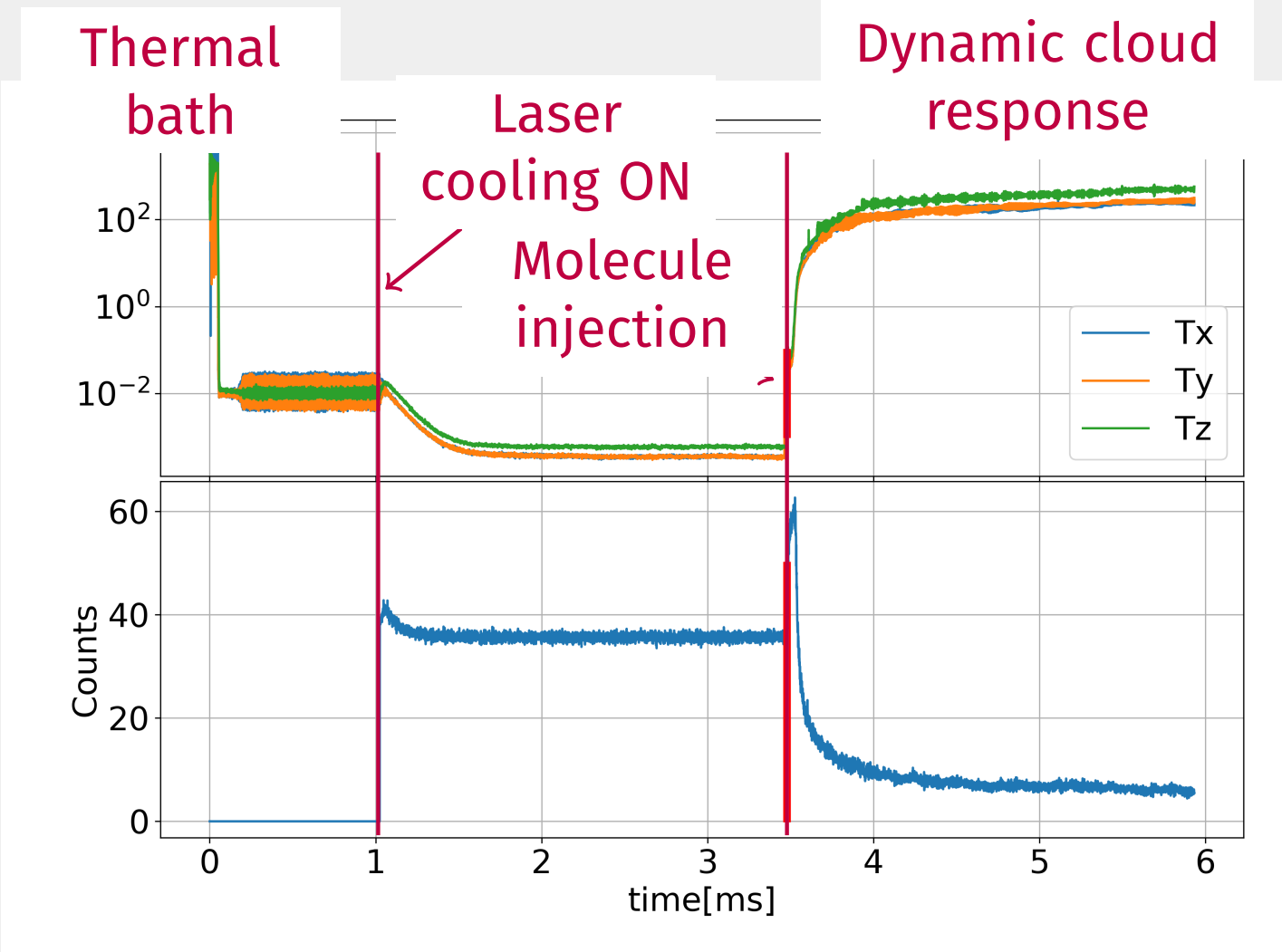


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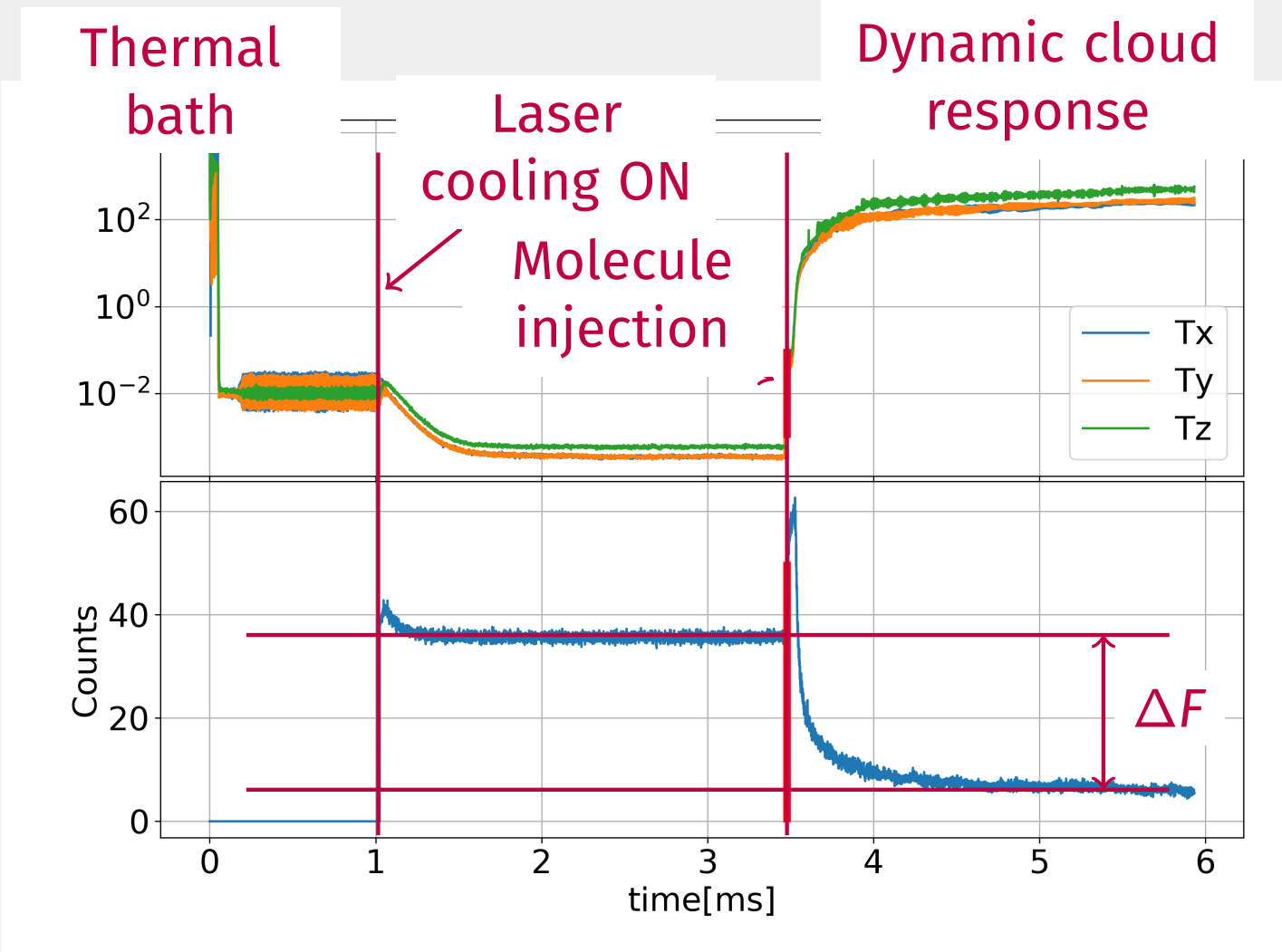


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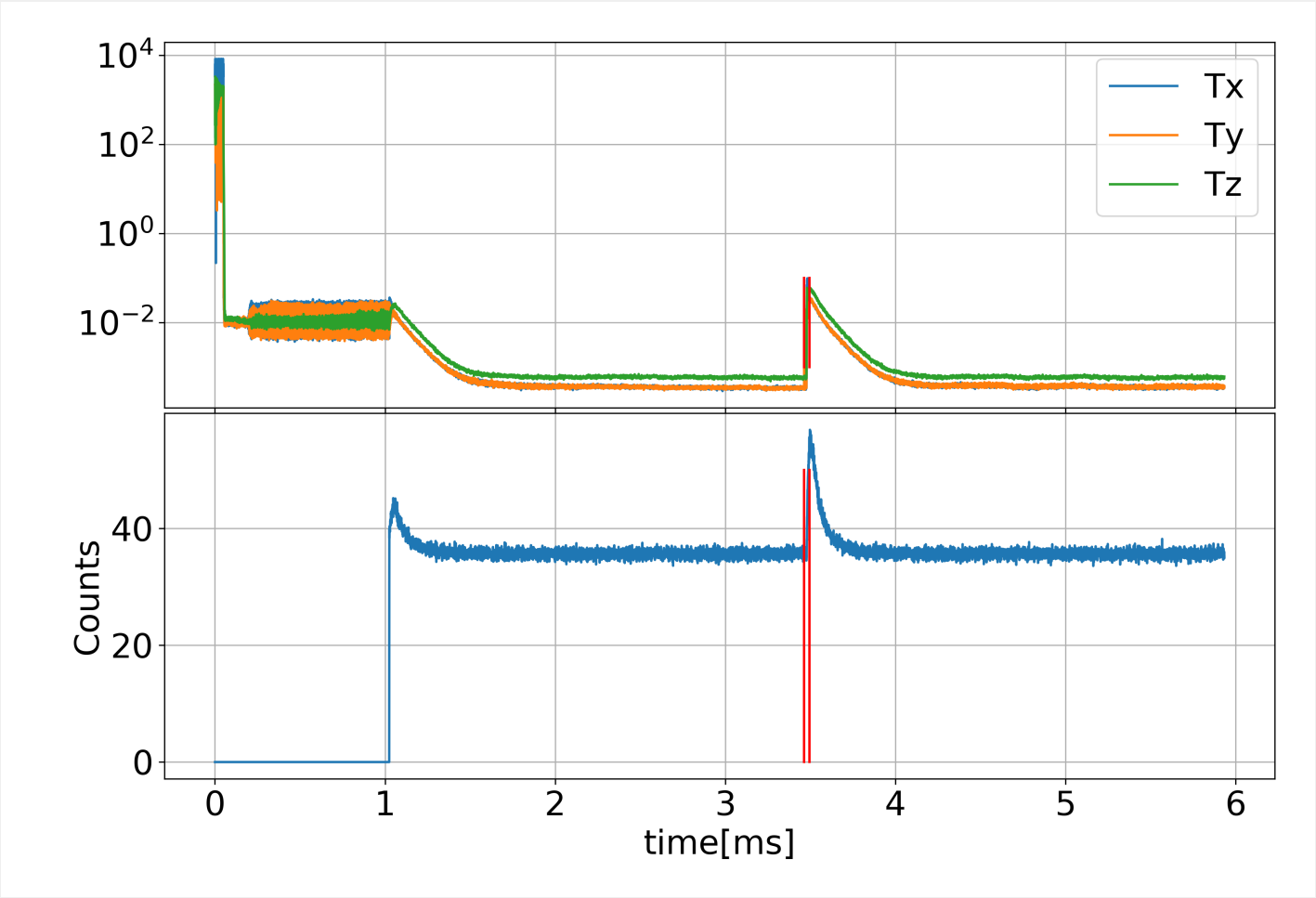
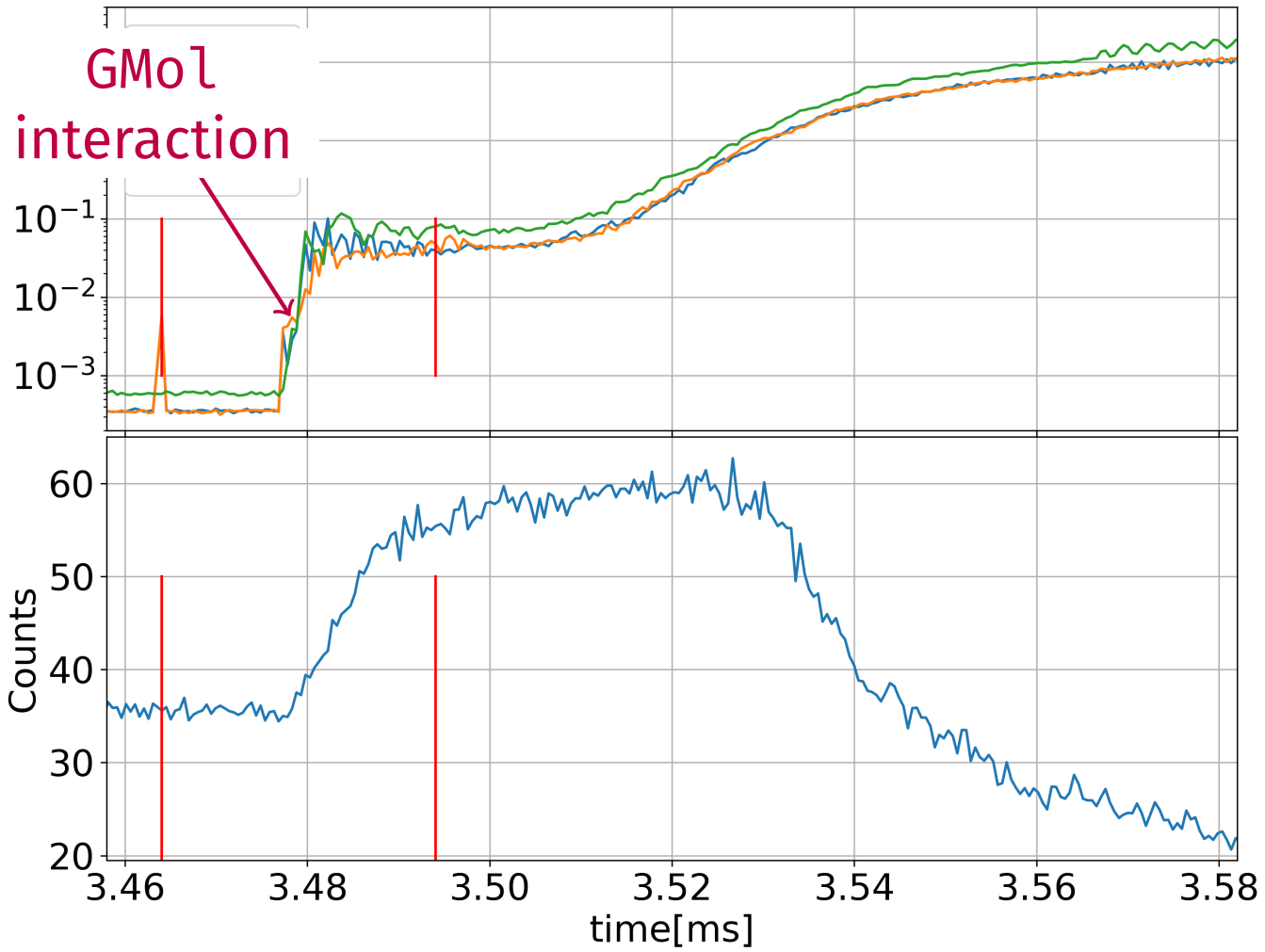



Fluorescence variation not significant enough to provide a molecule detection.

# Detection signal




Detection signal (focus on the post-injection dynamic).

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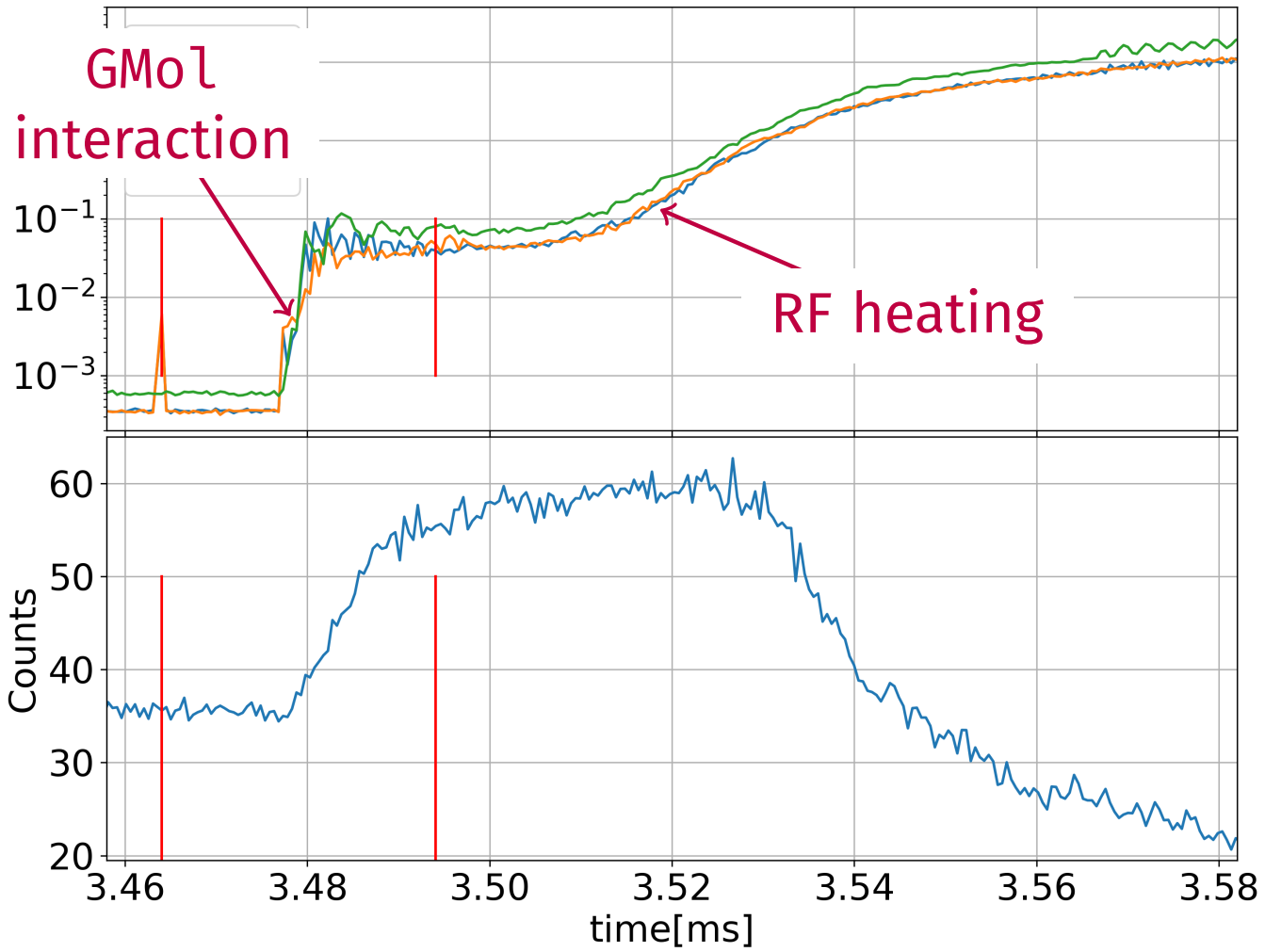


Detection signal (focus on the post-injection dynamic).

# GMol $\rightarrow$ $Ca^{+}$ Interaction Simulation

## Systematic study

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> Atoms

$n_{ionsC_a^+}$ ✗ 1024 ions

$m_{GMol}$ ✗ 1 Mamu

$E_{GMol}$ ✗ 50 eV ($\approx 100 m/s$)

$q_{Mol}$ ✗ 1 C

> Voltages

$V_{RF}|q_r$ ✓

$V_{ST}|a_r$ ✗ 0 V

$U_{DC}|a_z$ ✓

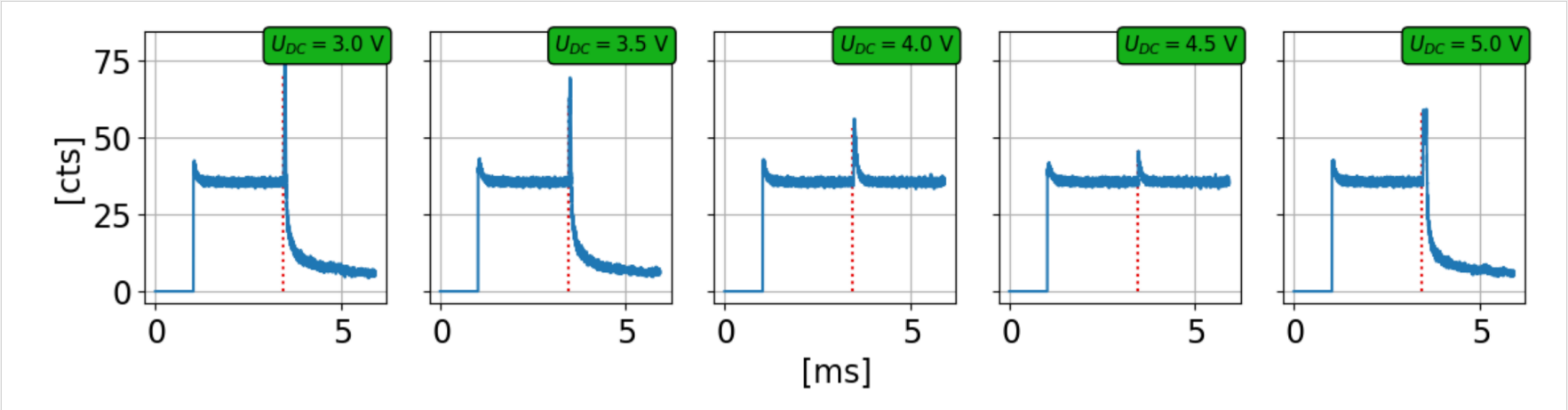
> Simulation parameters ✗

> Laser

**detuning** ✗ -Γ @ 397nm

**saturation** ✗ $S = 1$

# Systematic study




Fluorescence progression for different axial voltages. Molecular mass 1 Mamu.

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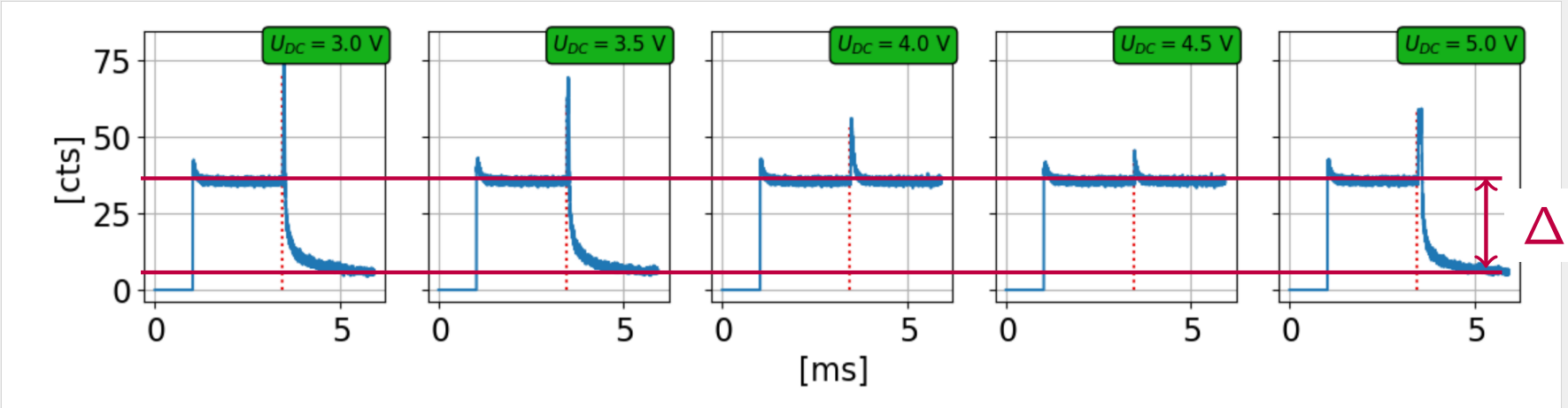


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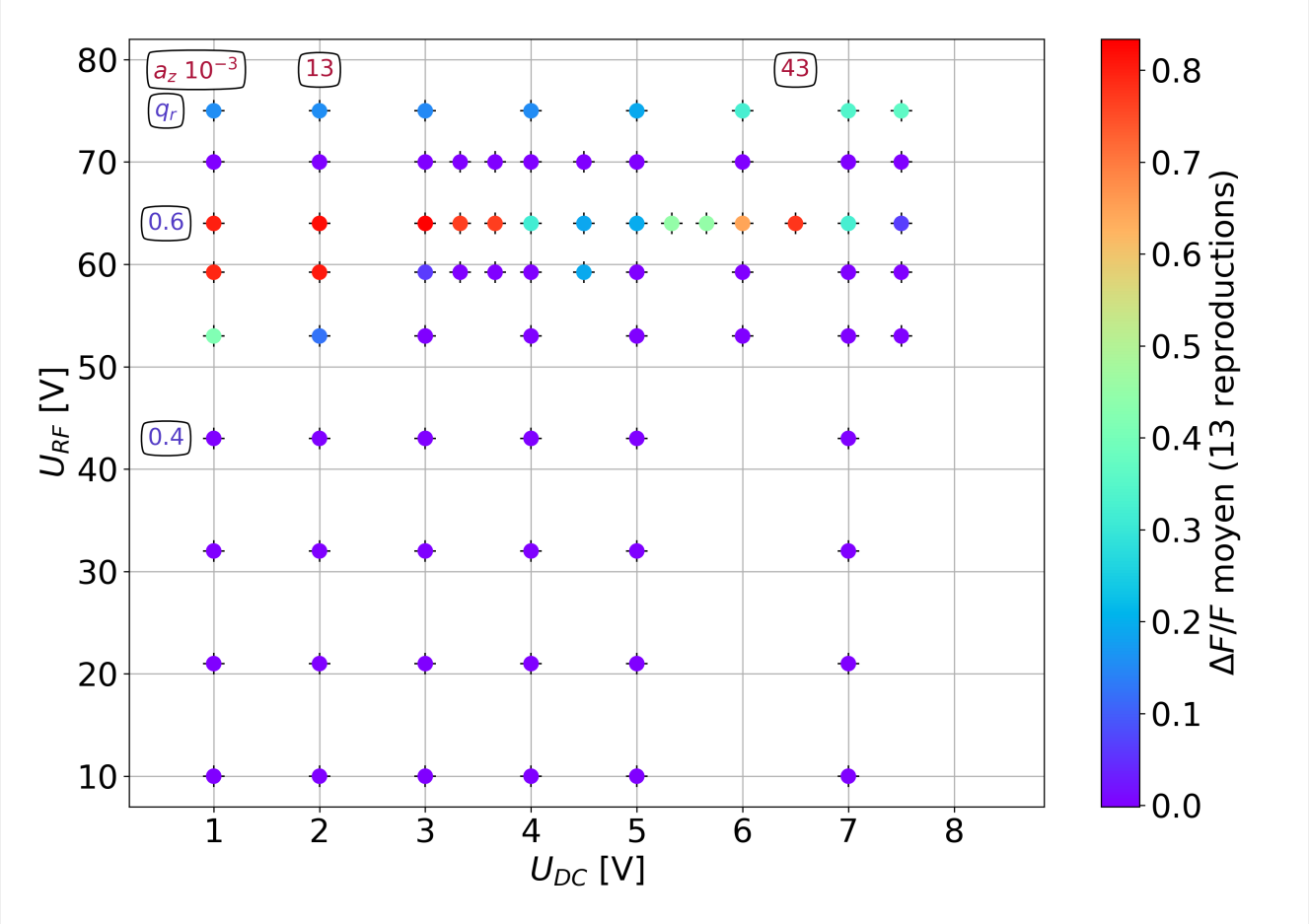
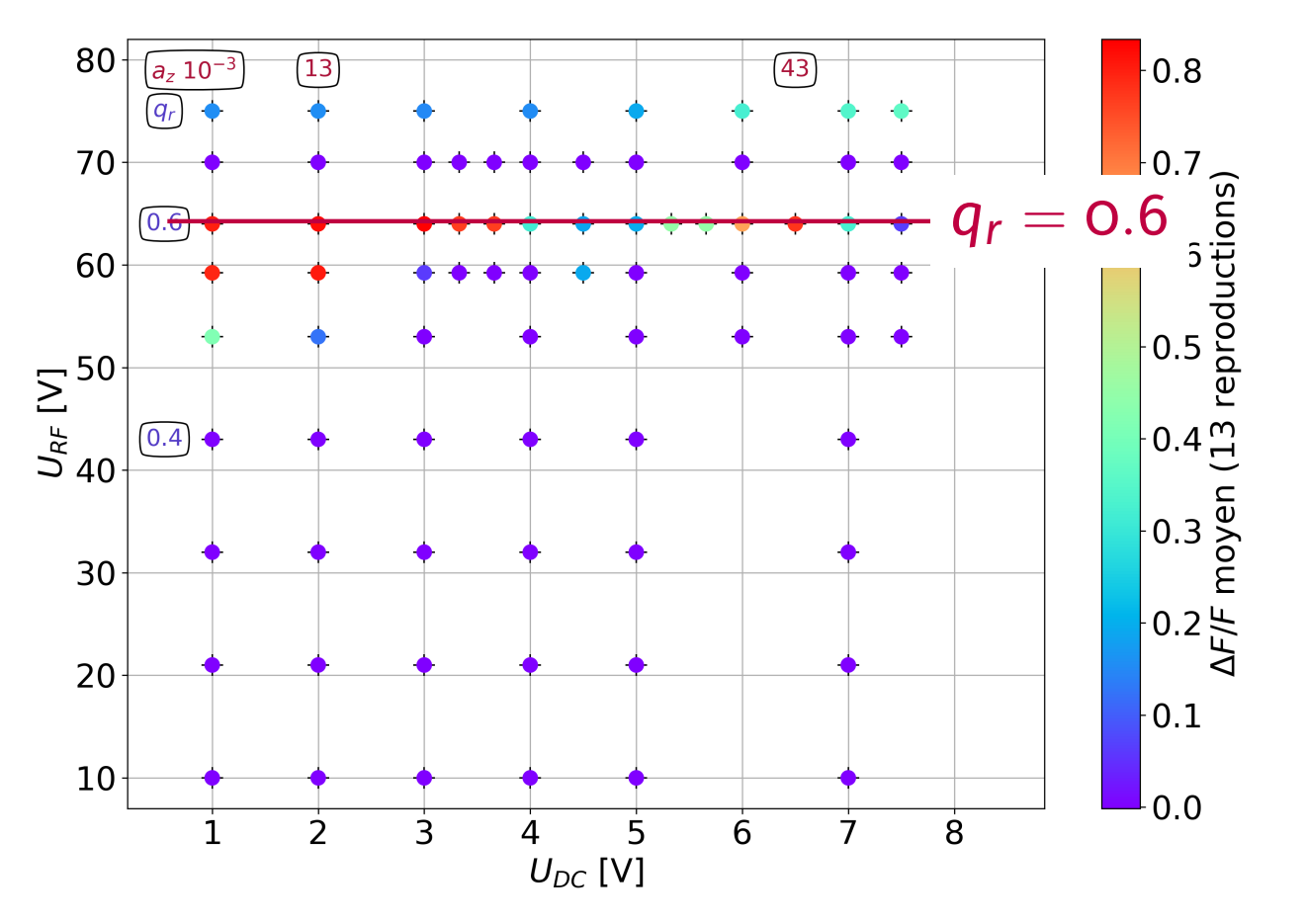



Detection efficiency as the relative fluorescence variation for different values of two parameters.

# Systematic study

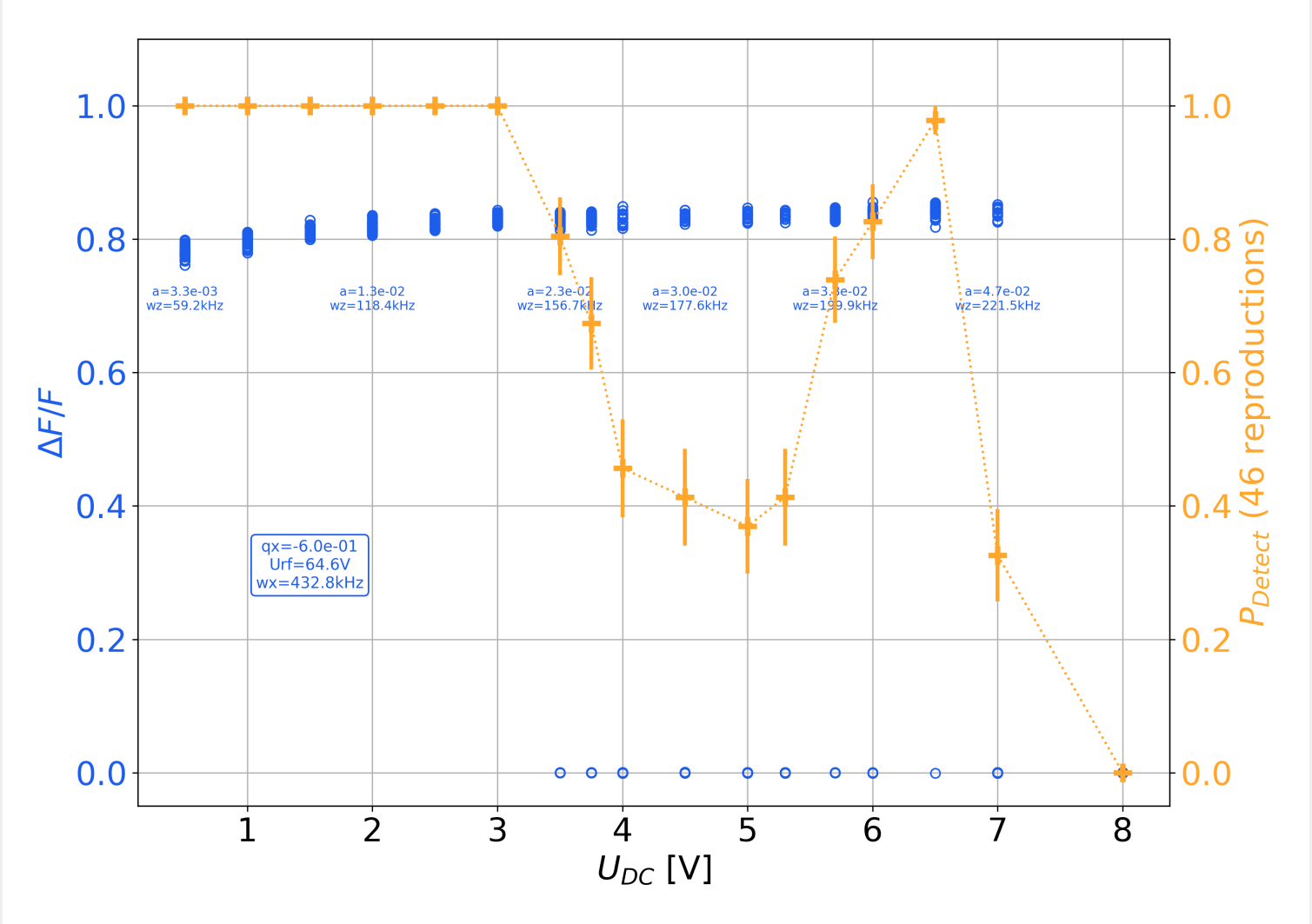



Detection efficiency as the relative fluorescence variation for different values of two parameters.

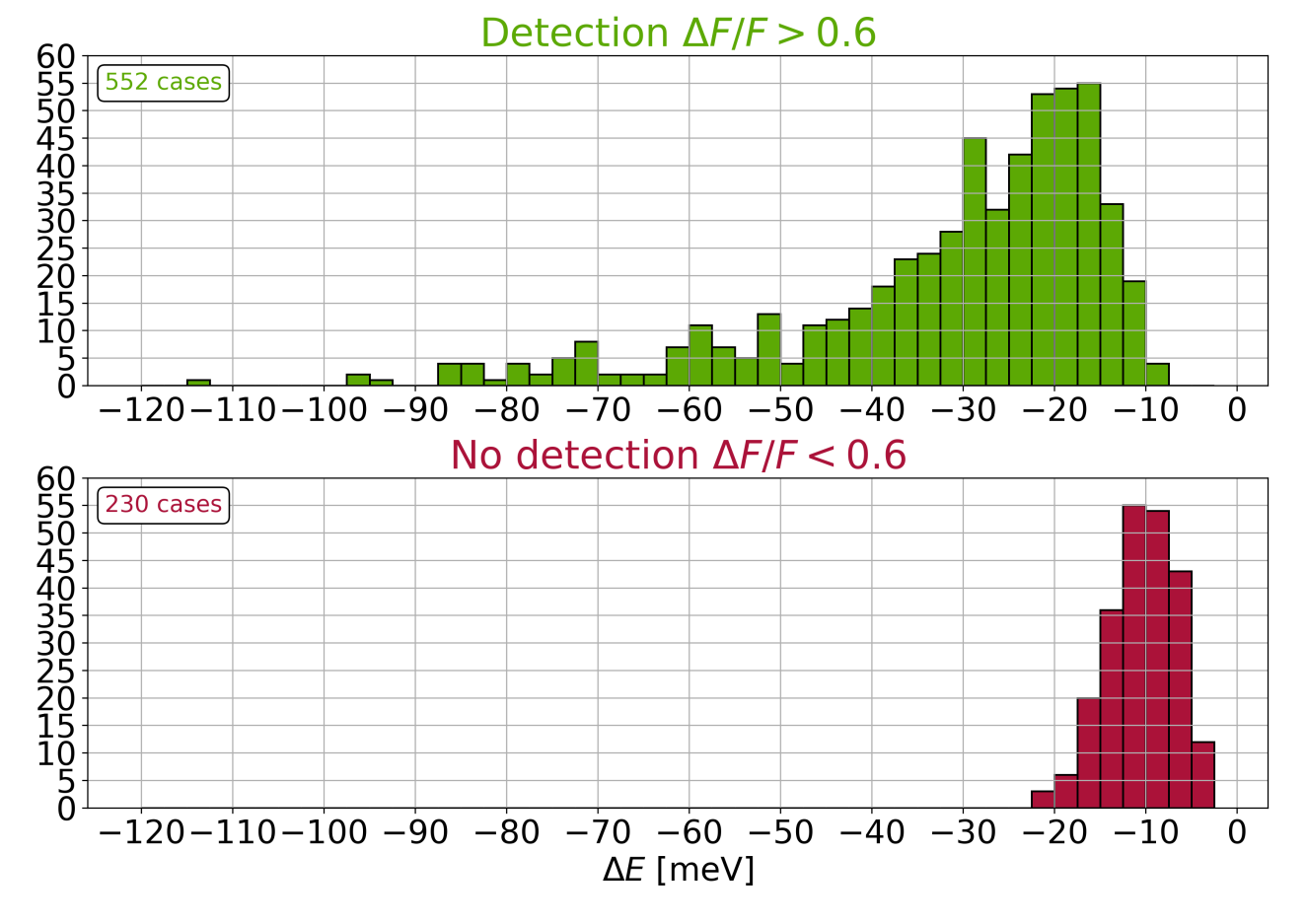
# GMol $\rightarrow$ Ca$^{+}$
# INTERACTION SIMULATION

## FOCUS ON THE $q_r = 0.6$ DATA

# Statistical analysis for fluorescence progression

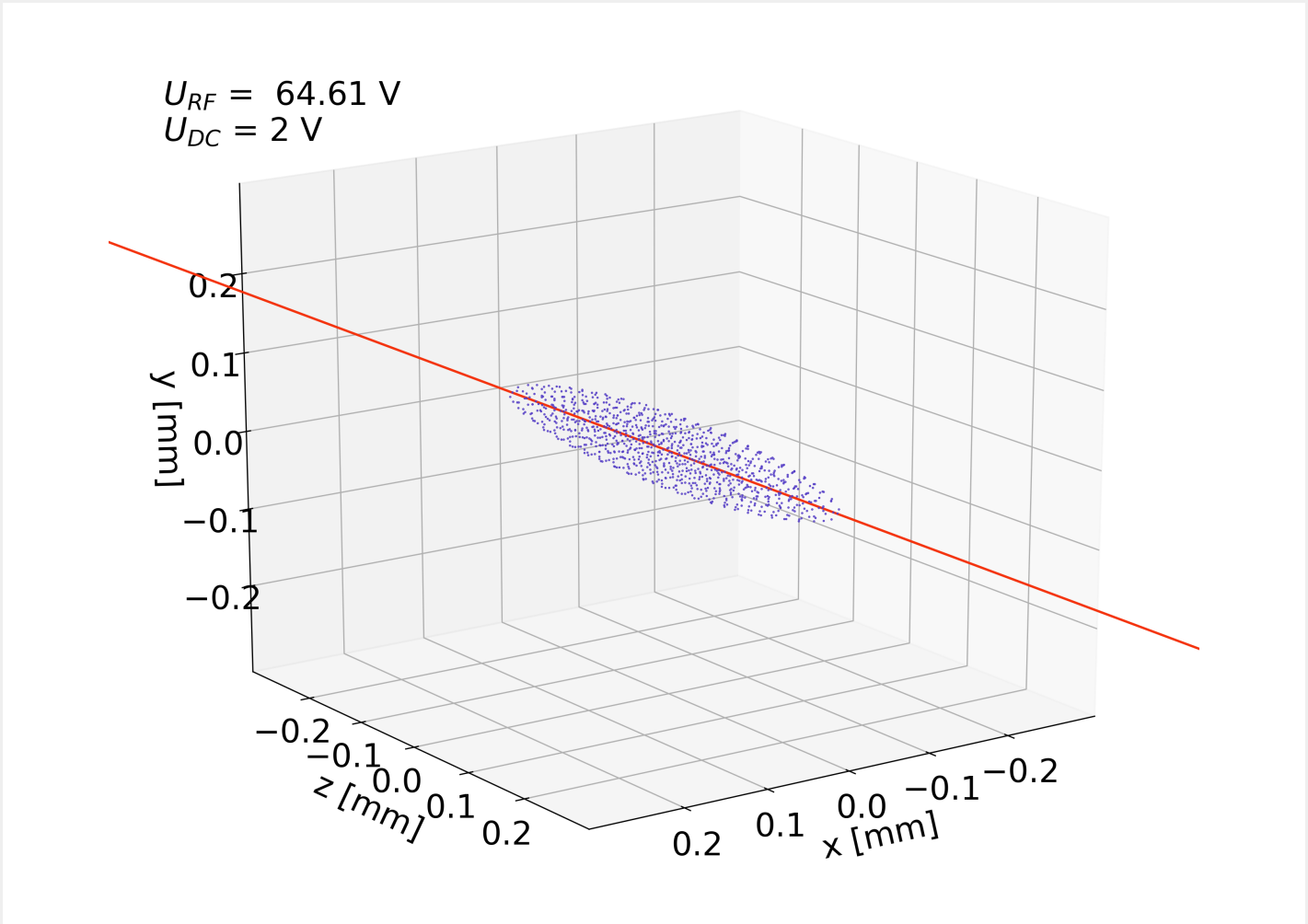


# Molecular ion energy loss




Energy loss histogram for molecular ion after interaction with $Ca^+$ ion cloud.

# Molecular ion behaviour




Molecular ion trajectory inside the $Ca^+$ ion cloud.

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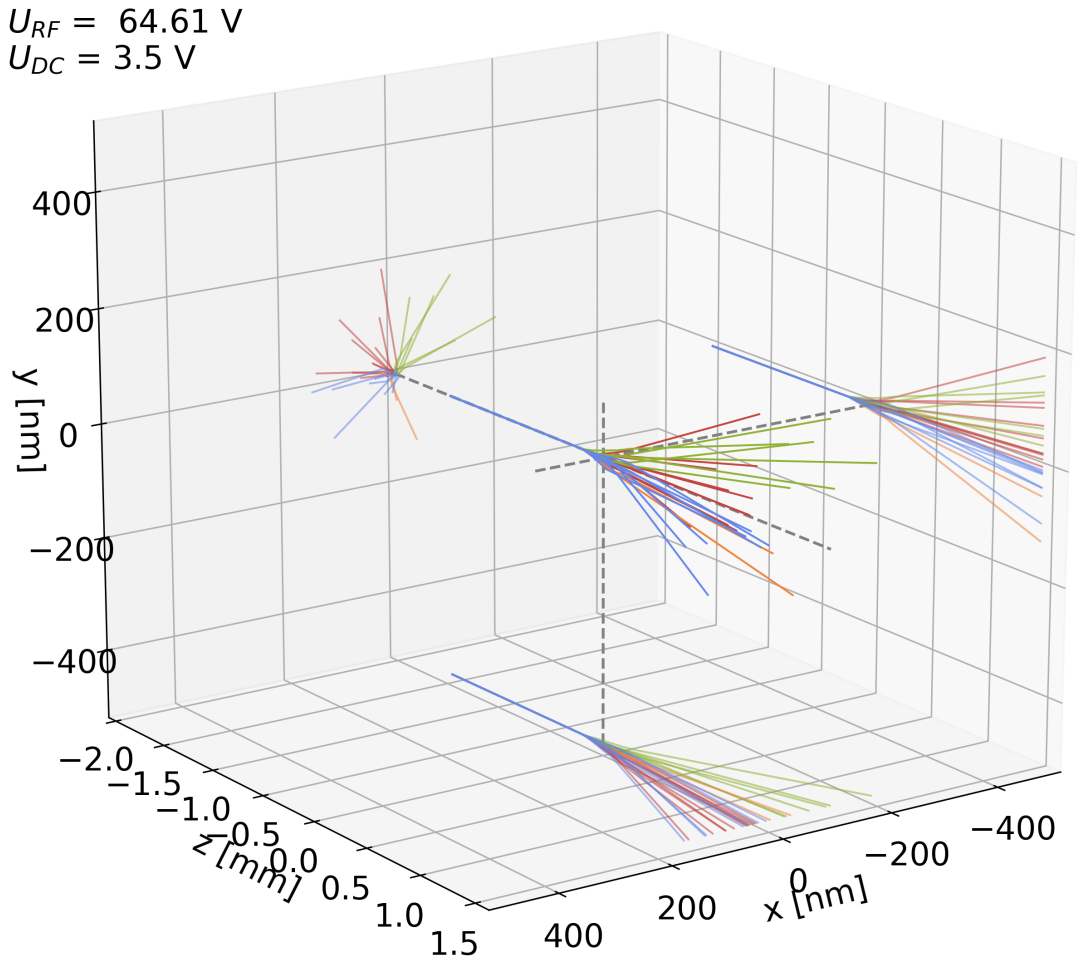
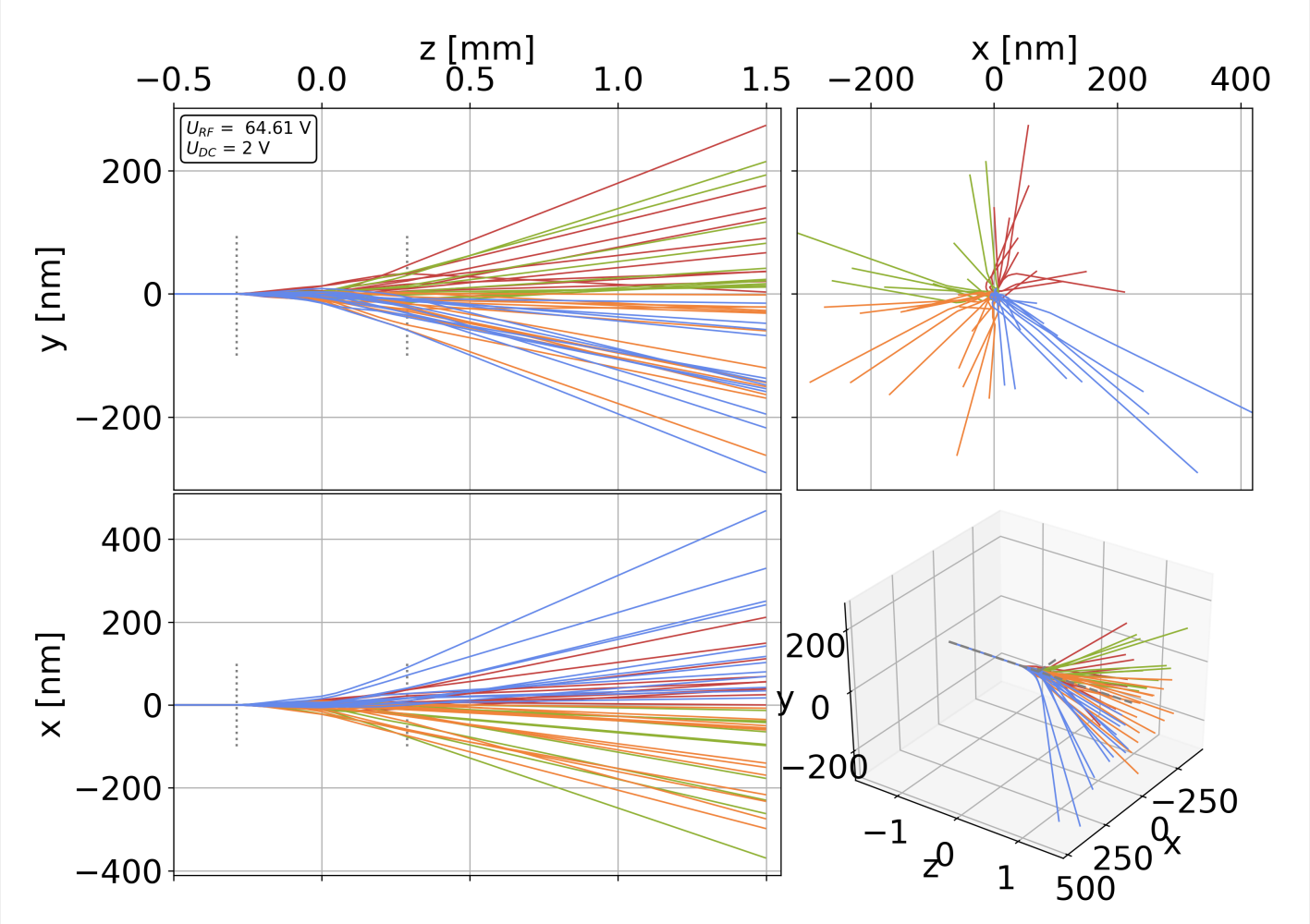
- Better comprehension of the experimental parameters influence, thanks to simulations *and* experiments;
- Necessity to work on other elements such as laser cooling, `GMol` incidence, energy charge and mass;
- Get closer to nominal operating conditions : increase molecular ion mass, produce a detection via $Ca^+$ ion cloud.

# Molecular ion behaviour



# Molecular ion behaviour




Detailed trajectories for all reproduction of one condition.