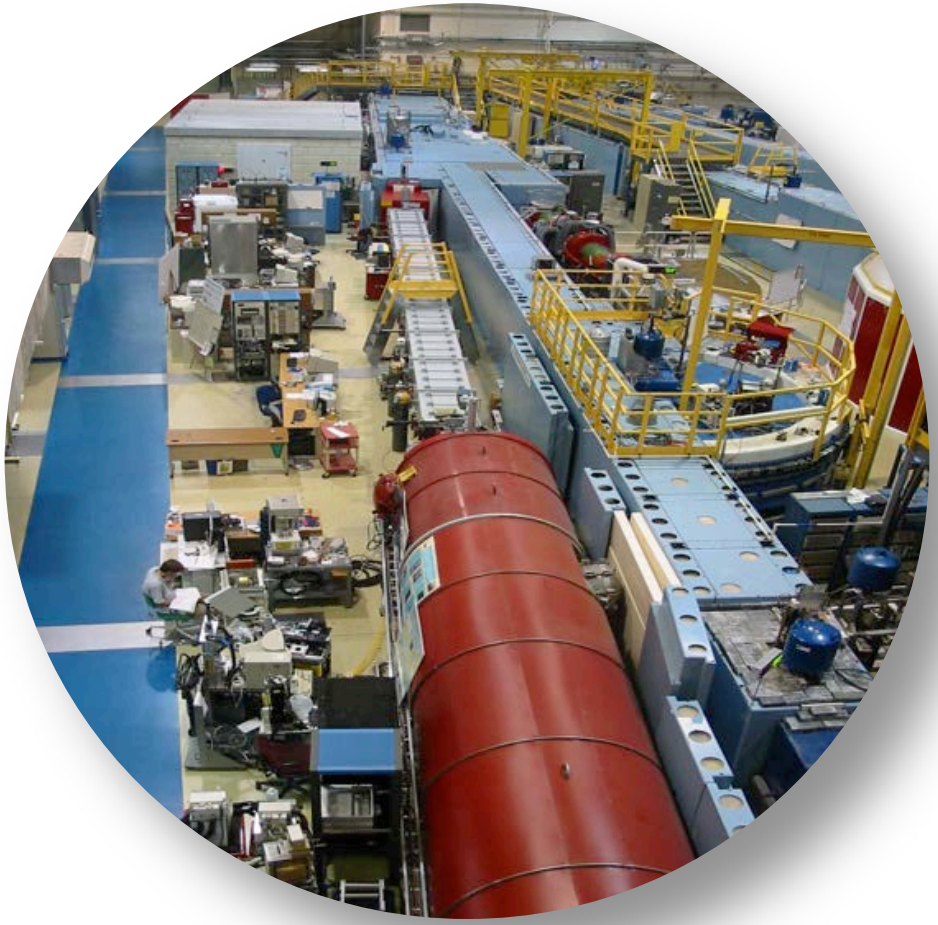
# SANS and USANS Experiment Planning



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# Why Plan the Experiment?

- Neutrons are an expensive resource, so we don't want to waste them.
- Deuterated chemicals can be expensive, so we don't want to waste them!

| | |
|---|---|
| Protonated SDS (≥99% SDS) | $1.56/gram |
| Deuterated SDS | $425.00/gram |

- We want to make sure that we can get the best possible data (and most useful) before we invest time, money, travel, (tears?) into sample preparation.

# Scattering Length Density (SLD)

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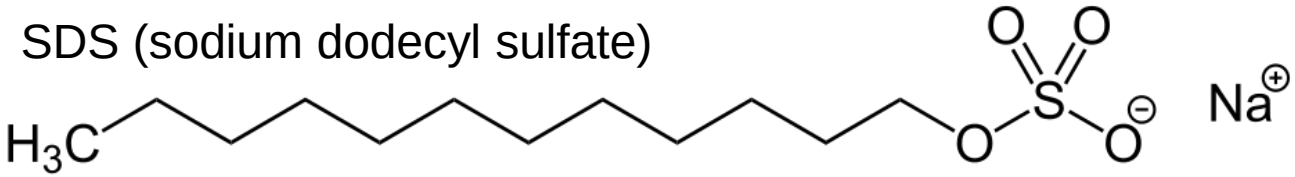
"Bound coherent scattering length"

$$\rho = \frac{1}{V_m} \sum_{i=1}^{n} b_{c,i}$$

Usually given in units of inverse squared Angstrom or centimeter ($A^{-2}$ or $cm^{-2}$).

So let's calculate the SLD of SDS:

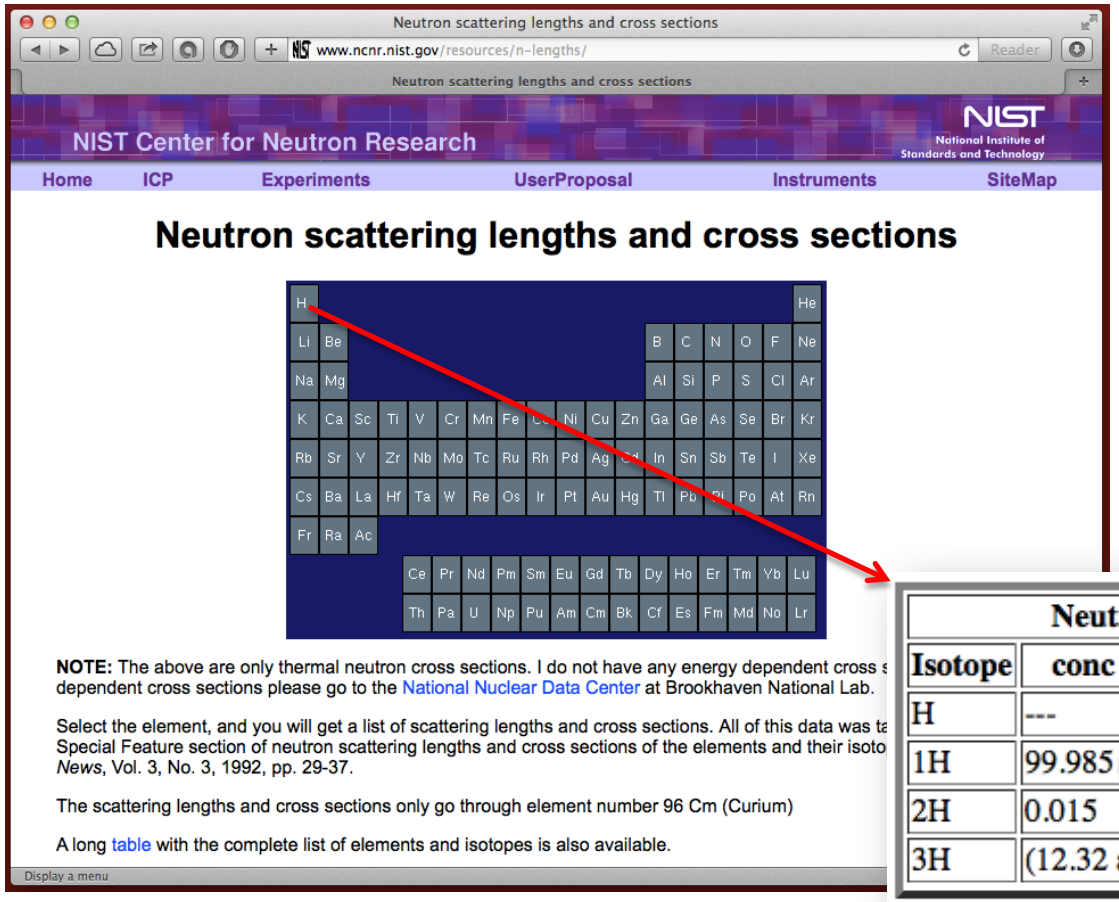
SDS (sodium dodecyl sulfate)




**$NaC_{12}H_{25}SO_4$**

# Scattering Length Density – The Long Way

## http://www.ncnr.nist.gov/n-lengths




$$\rho = \frac{1}{V_m} \sum_{i=1}^{n} b_{c,i}$$

**Neutron scattering lengths and cross sections**

| Isotope | conc | Coh b | Inc b | Coh xs | Inc xs | Scatt xs | Abs xs |
|---|---|---|---|---|---|---|---|
| H | --- | -3.7390 | -- | 1.7568 | 80.26 | 82.02 | 0.3326 |
| 1H | 99.985 | -3.7406 | 25.274 | 1.7583 | 80.27 | 82.03 | 0.3326 |
| 2H | 0.015 | 6.671 | 4.04 | 5.592 | 2.05 | 7.64 | 0.000519 |
| 3H | (12.32 a) | 4.792 | -1.04 | 2.89 | 0.14 | 3.03 | 0 |

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$$\rho = \frac{1}{V_m}\sum_{i=1}^{n} b_{c,i}$$

**1 fm = 1 fermi = $10^{-5}$ Angstrom**

$$\rho = \frac{1}{(474.28\ \text{Å}^3)}\left\{3.63 + 12(6.65) + 25(-3.74) + 2.80 + 4(5.80)\right\}\ \text{fm}$$

**Na C H S O**

**Volume of 1 SDS molecule calculated from mass density**

**$= 3.36 \times 10^{-7}\ \text{A}^{-2}$**

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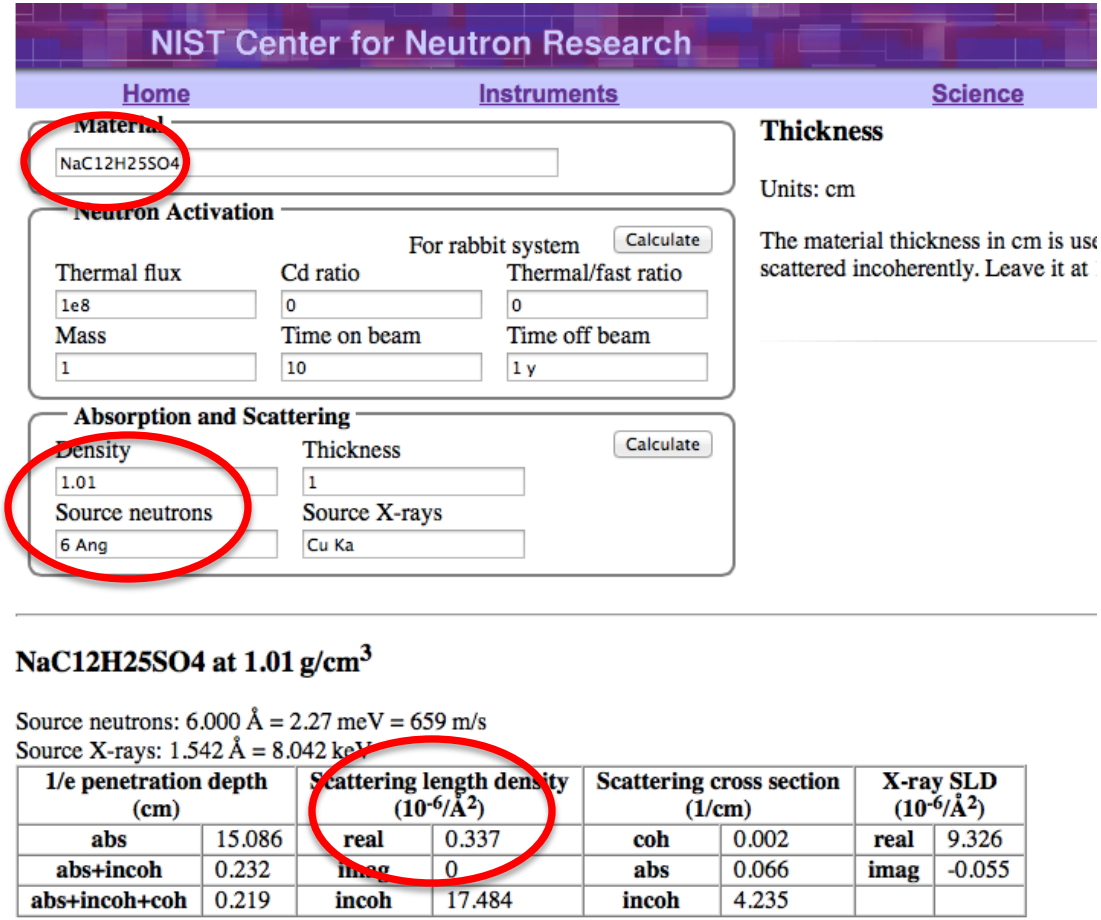
# Scattering Length Density – The Easy Way

**http://www.ncnr.nist.gov/resources/activation**




**= 3.37 x $10^{-7}$ $A^{-2}$**

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# Scattering Length Density – The Easy Way

**http://www.ncnr.nist.gov/resources/activation**

**D2O at 1.10 g/cm$^3$**

Source neutrons: 6.000 Å = 2.27 meV = 659 m/s
Source X-rays: 1.542 Å = 8.042 keV

| 1/e penetration depth (cm) | | Scattering length density ($10^{-6}$/Å$^2$) | | Scattering cross section (1/cm) | | X-ray SLD ($10^{-6}$/Å$^2$) | |
|---|---|---|---|---|---|---|---|
| **abs** | 7377.775 | **real** | 6.335 | **coh** | 0.508 | **real** | 9.369 |
| **abs+incoh** | 7.367 | **imag** | 0 | **abs** | 0.000 | **imag** | -0.031 |
| **abs+incoh+coh** | 1.549 | **incoh** | 3.272 | **incoh** | 0.136 | | |

Neutron transmission is 87.31% for 1 cm of sample (after absorption and incoherent scattering).
Transmitted flux is 8.731e+7 n/cm$^2$/s for a 1e8 n/cm$^2$/s beam.

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**NaC12H25SO4 at 1.01 g/cm$^3$**

Source neutrons: 6.000 Å = 2.27 meV = 659 m/s
Source X-rays: 1.542 Å = 8.042 keV

| 1/e penetration depth (cm) | | Scattering length density ($10^{-6}$/Å$^2$) | | Scattering cross section (1/cm) | | X-ray SLD ($10^{-6}$/Å$^2$) | |
|---|---|---|---|---|---|---|---|
| **abs** | 15.086 | **real** | 0.337 | **coh** | 0.002 | **real** | 9.326 |
| **abs+incoh** | 0.232 | **imag** | 0 | **abs** | 0.066 | **imag** | -0.055 |
| **abs+incoh+coh** | 0.219 | **incoh** | 17.484 | **incoh** | 4.235 | | |

Neutron transmission is 1.35% for 1 cm of sample (after absorption and incoherent scattering).
Transmitted flux is 1.354e+6 n/cm$^2$/s for a 1e8 n/cm$^2$/s beam.

# Estimating Scattering

# Estimating Scattering in Igor Pro

**For uniform ellipsoidal micelles in a solvent:**

$$I(q) \propto \phi(\rho_{ell} - \rho_{solv})^2 \cancel{F(q)} + Bkg$$

**Scattered Intensity**

**Volume Fraction**

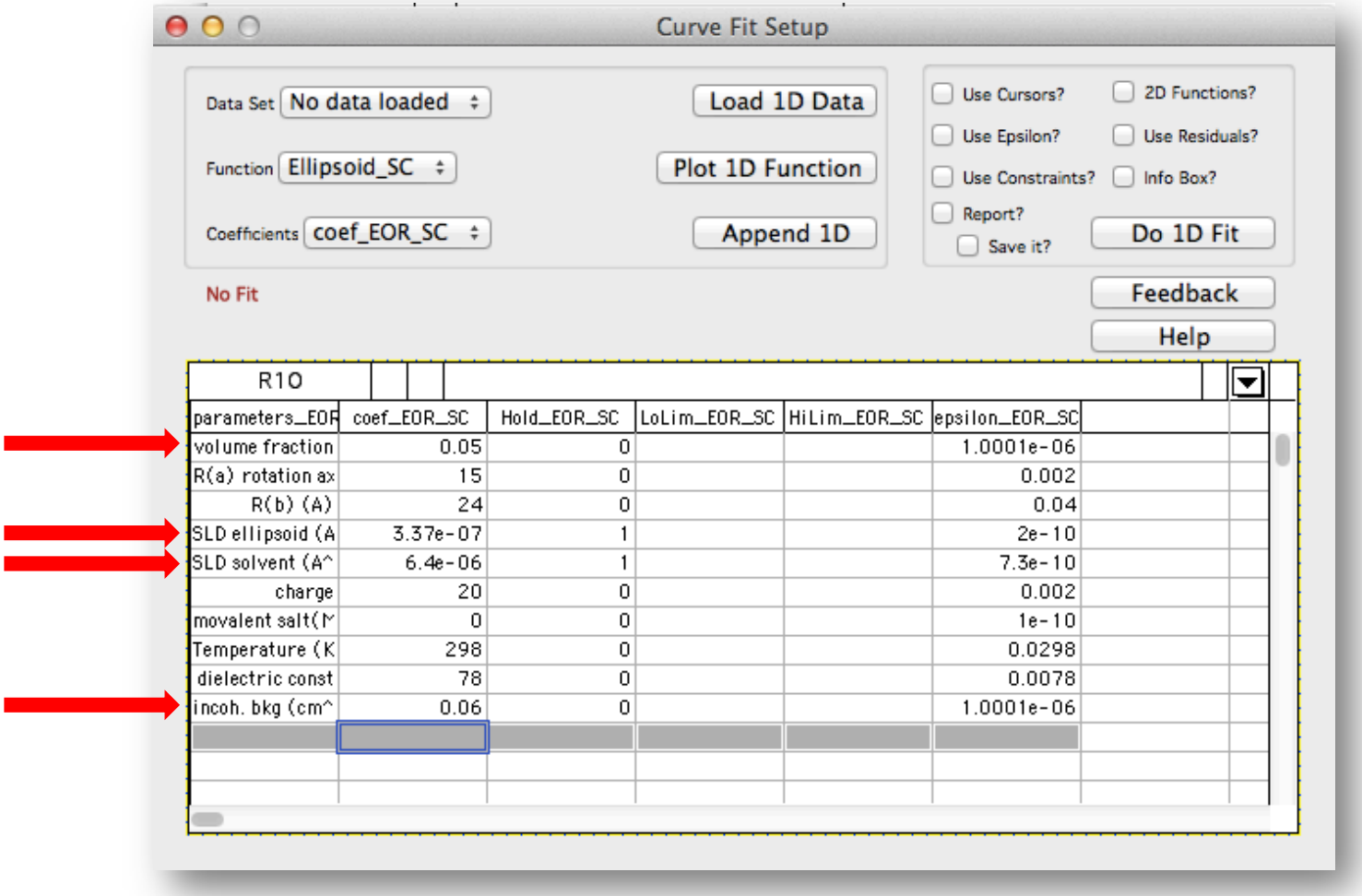
**Difference in SLDs or the "Contrast"**

**Incoherent Background "noise" from Hydrogen (primarily)**

**What do we want for "good" data?**

- **Large contrast between micelle & solvent, lots of sample, and low background.**

# Estimating Scattering in Igor Pro




**Good rule of thumb for incoherent background (1 mm sample cell):**

- 0.06 $cm^{-1}$ for $D_2O$ as solvent
- 1.00 $cm^{-1}$ for $H_2O$ as solvent

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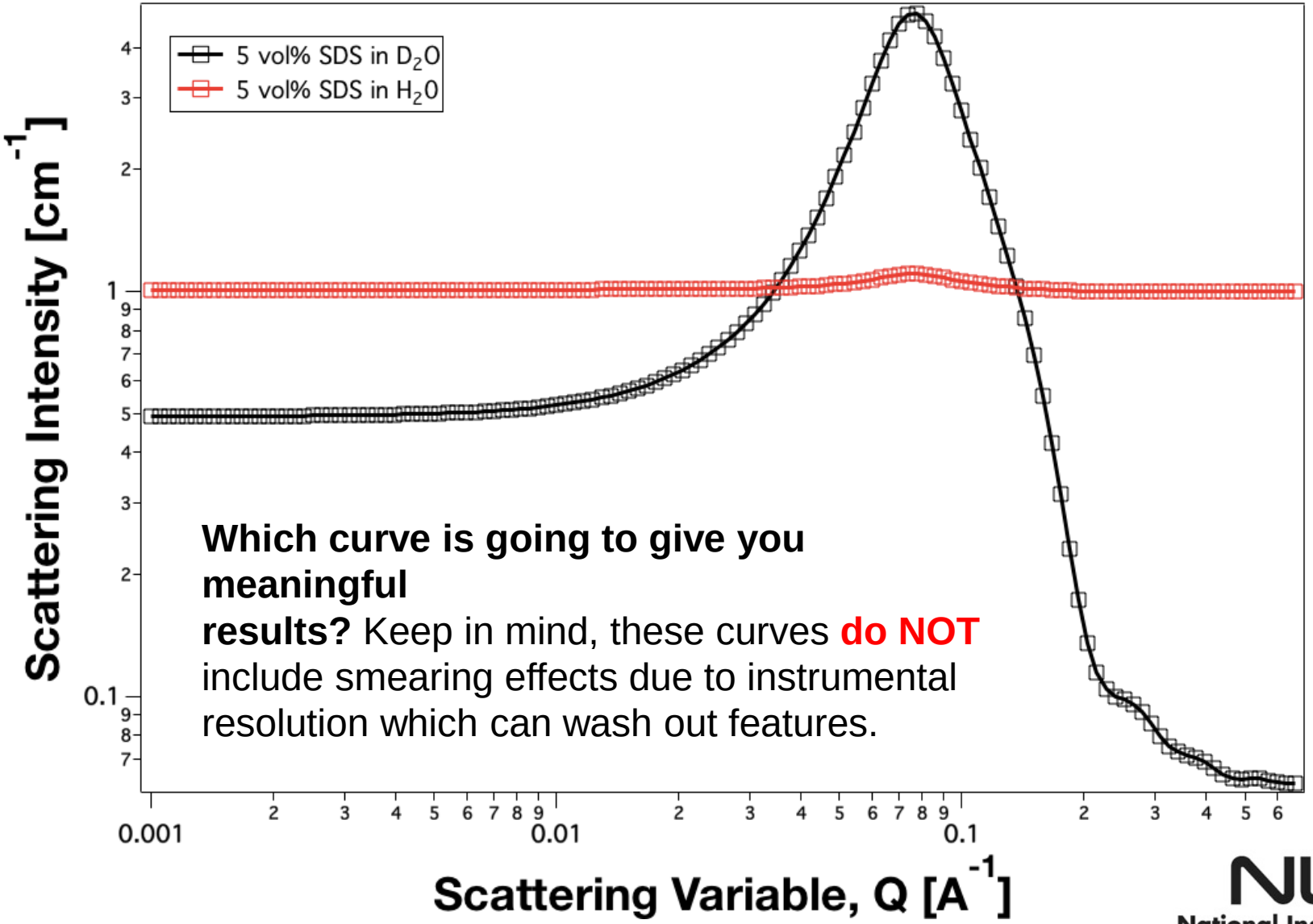
# Estimating Scattering in Igor Pro




**Which curve is going to give you meaningful results?** Keep in mind, these curves **do NOT** include smearing effects due to instrumental resolution which can wash out features.

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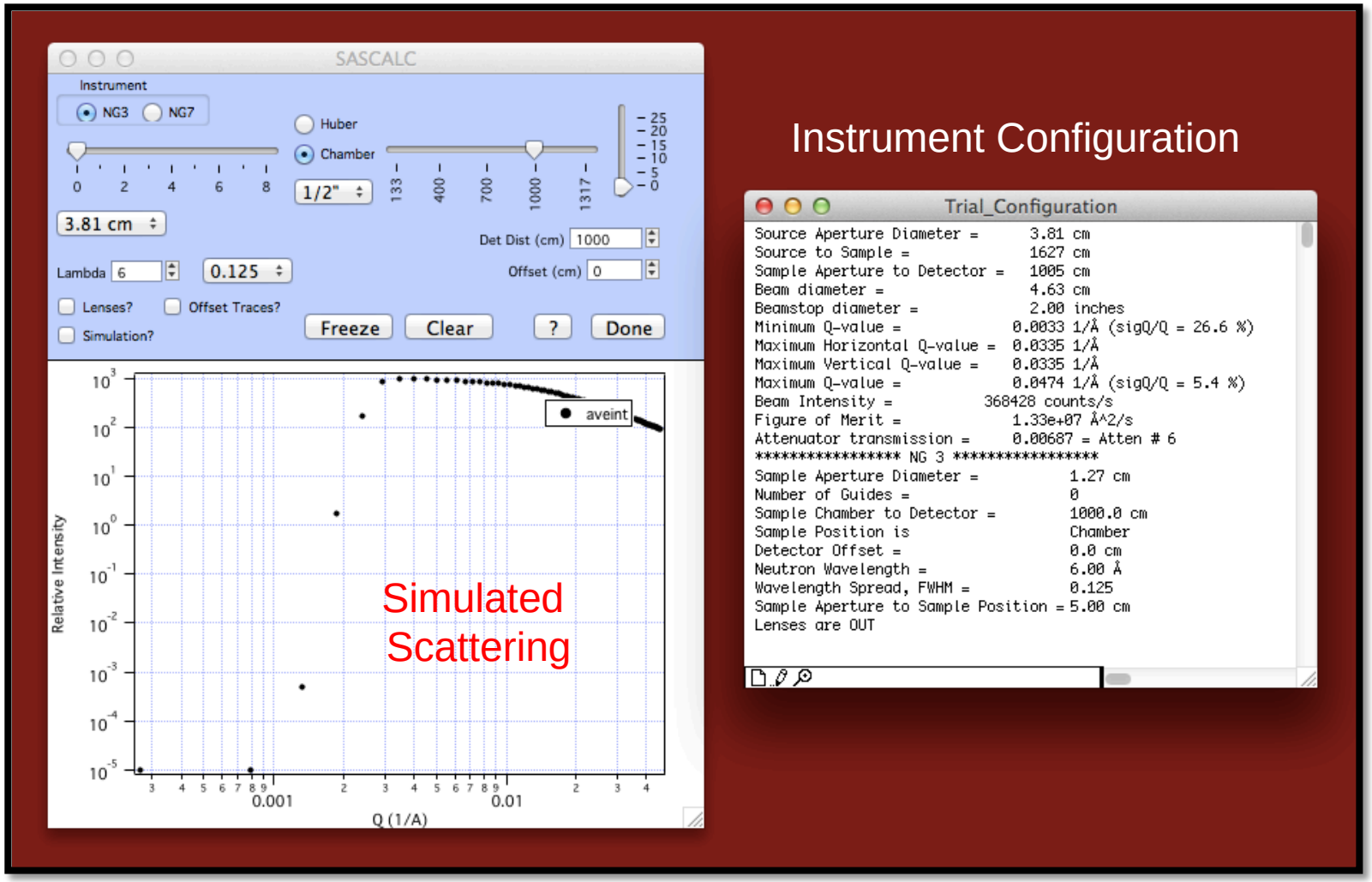
# Instrument Configuration / SANS Simulation (SASCALC)

# SASCALC (Inside Igor Pro Macros)

- Gives you a good feeling for what your scattering should look like.
- Allows you to configure the instrument to obtain best data.
- Estimate count times! Will you have to count for too long? Do you need fewer/more samples?
- Otherwise, you will use a “standard configuration” from your instrument scientist.

# SASCALC (Inside Igor Pro Macros)

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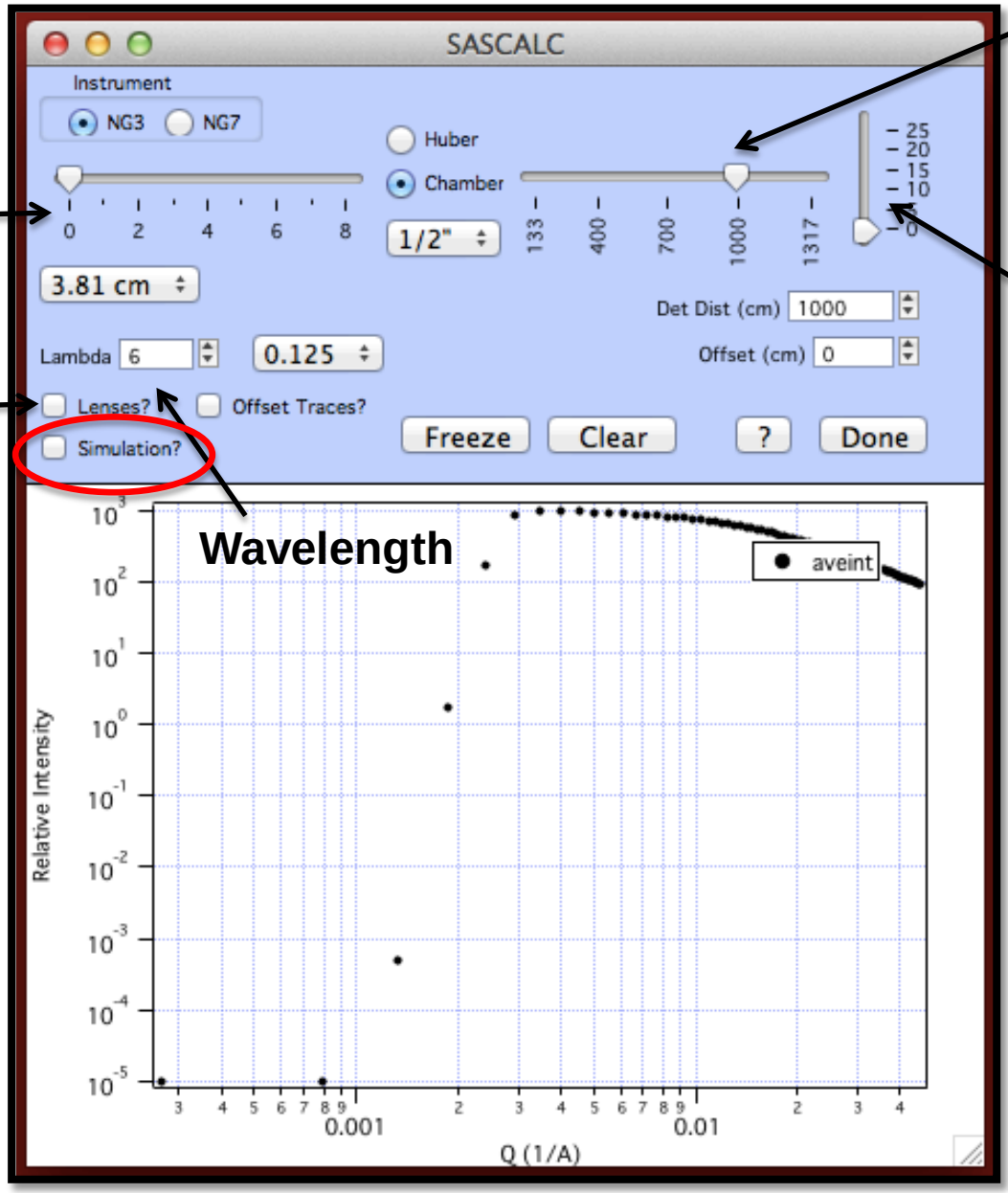
# SASCALC (Inside Igor Pro Macros)




**Detector Distance (cm)**

**# of Guides**

**Detector Offset (cm)**

**Use Focusing Lenses (13 m)?**

**Wavelength**

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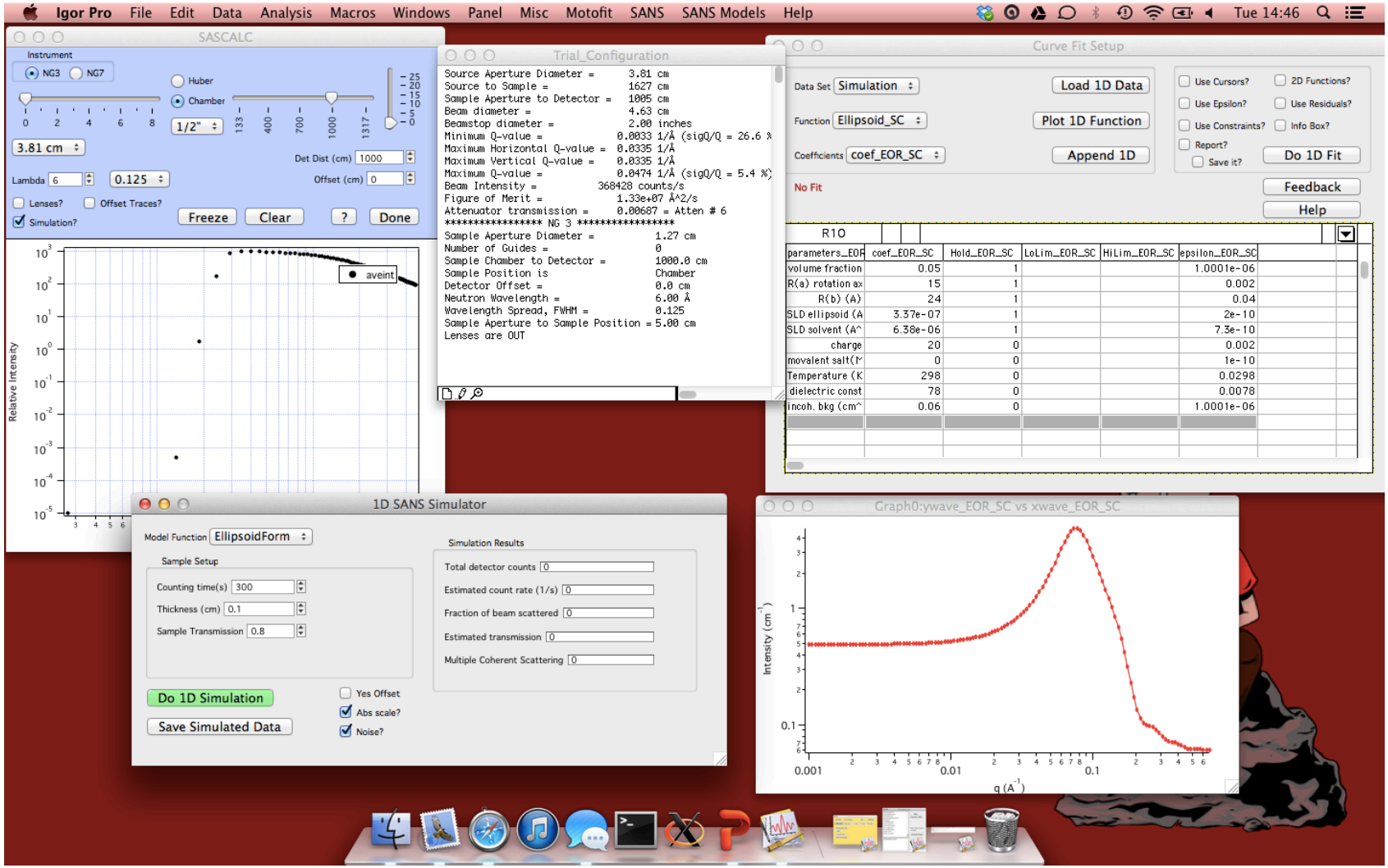
# SASCALC (Inside Igor Pro Macros)

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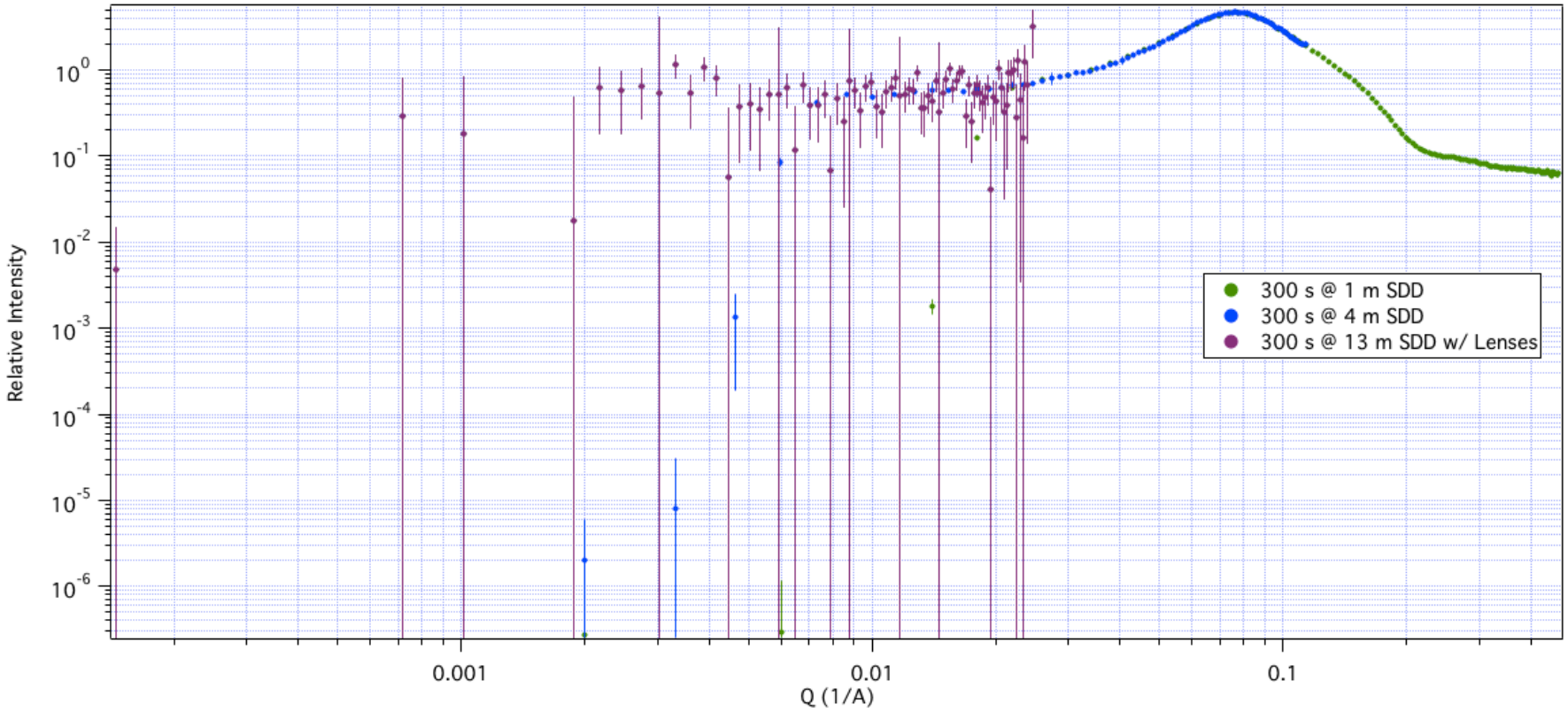
# SASCALC (Inside Igor Pro Macros)

**Counting for 300 s at each detector distance:**

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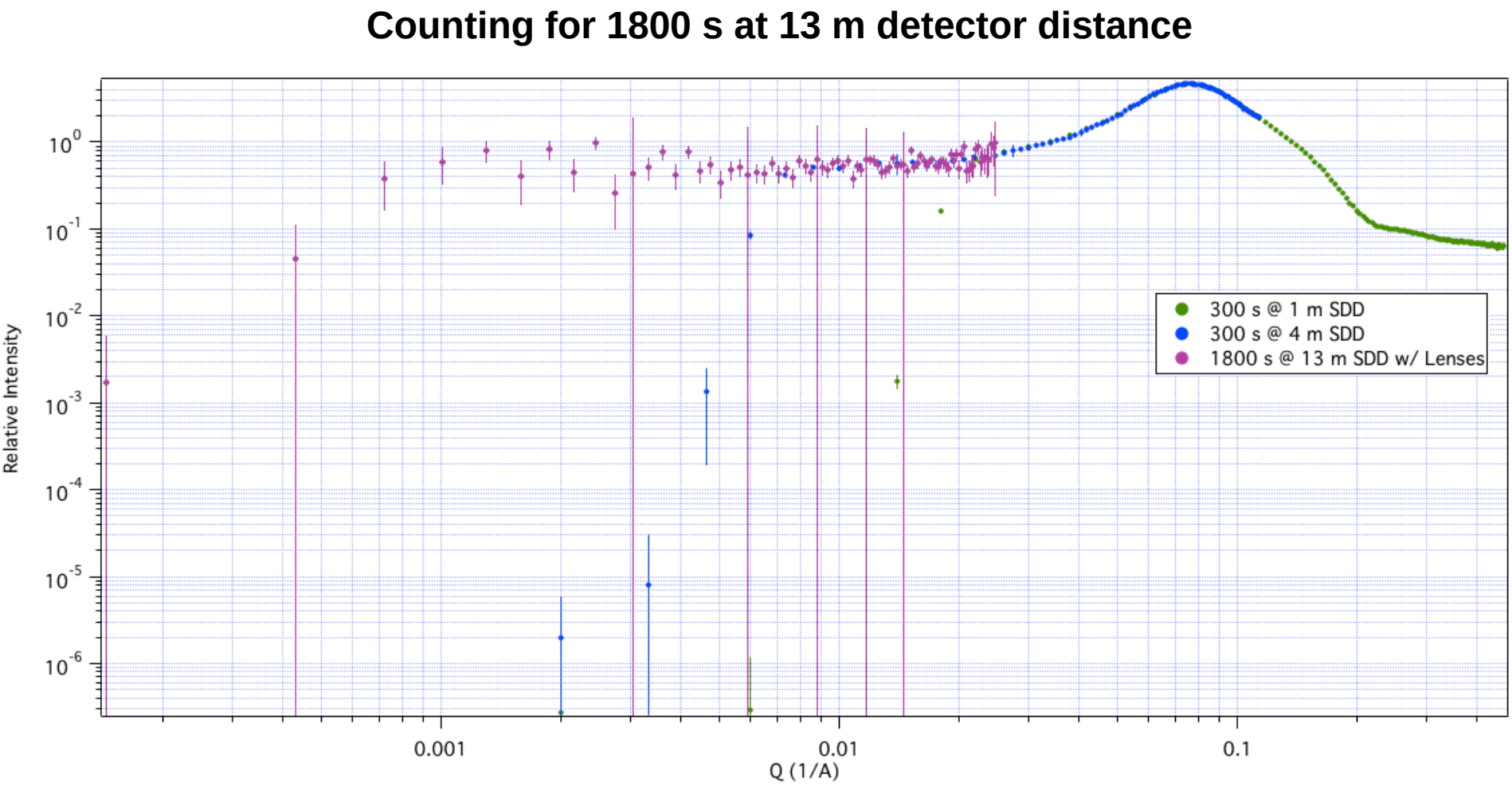
# SASCALC (Inside Igor Pro Macros)

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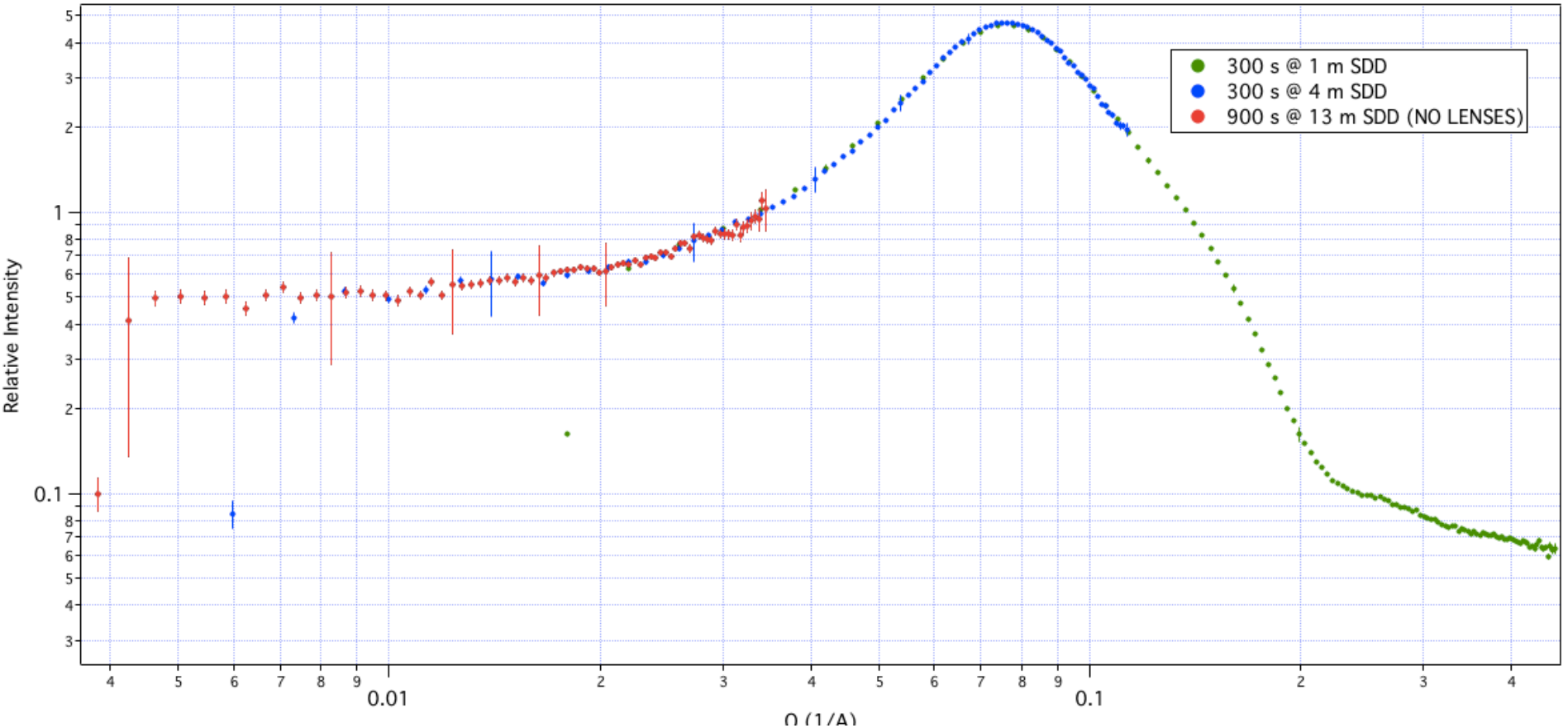
# SASCALC (Inside Igor Pro Macros)

**Counting for 900 s at 13 m detector distance (NO LENSES)**

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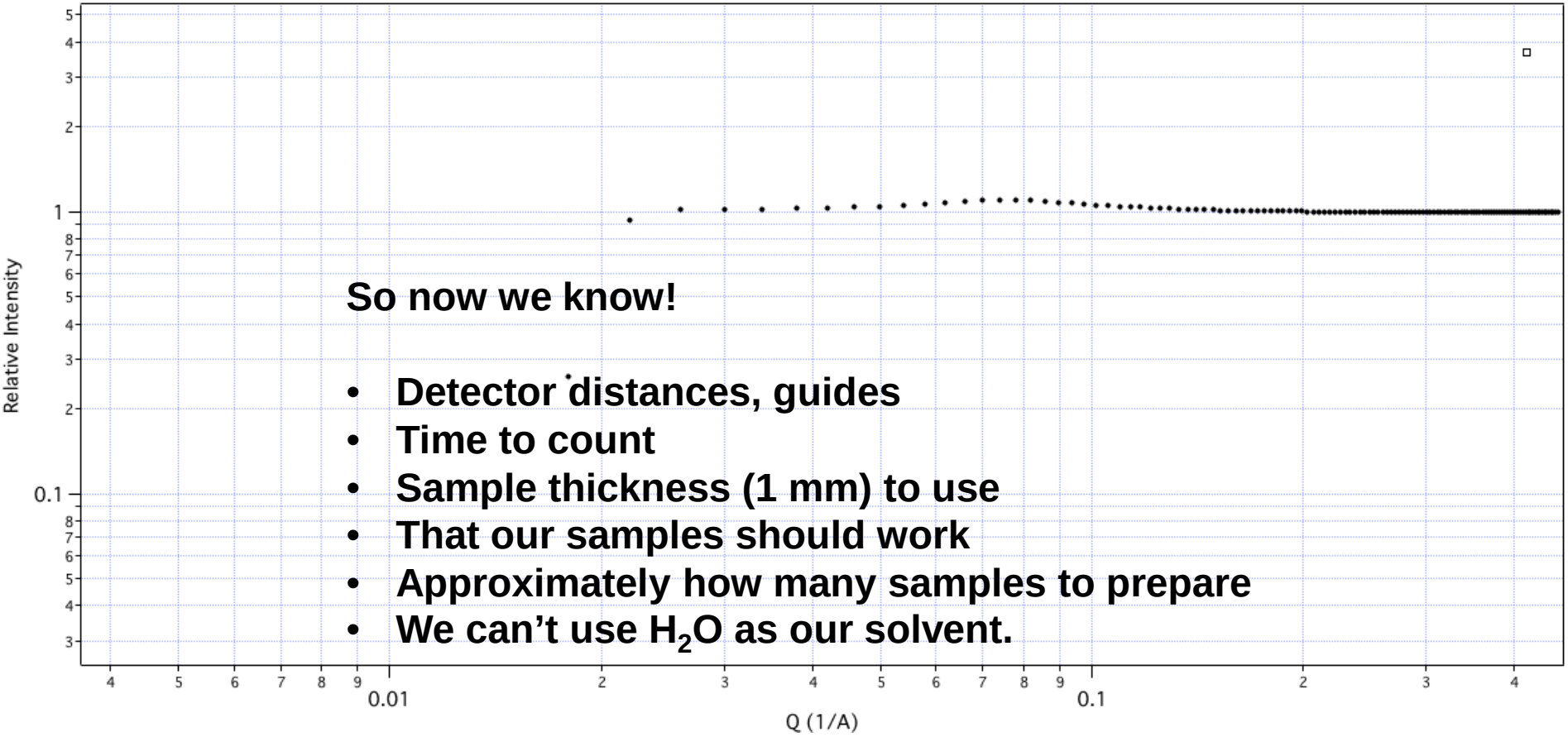
# SASCALC (Inside Igor Pro Macros)

**Counting for 1 day at 1 m detector distance in $H_2O$ – No signal essentially. Waste of neutrons/time/money.**



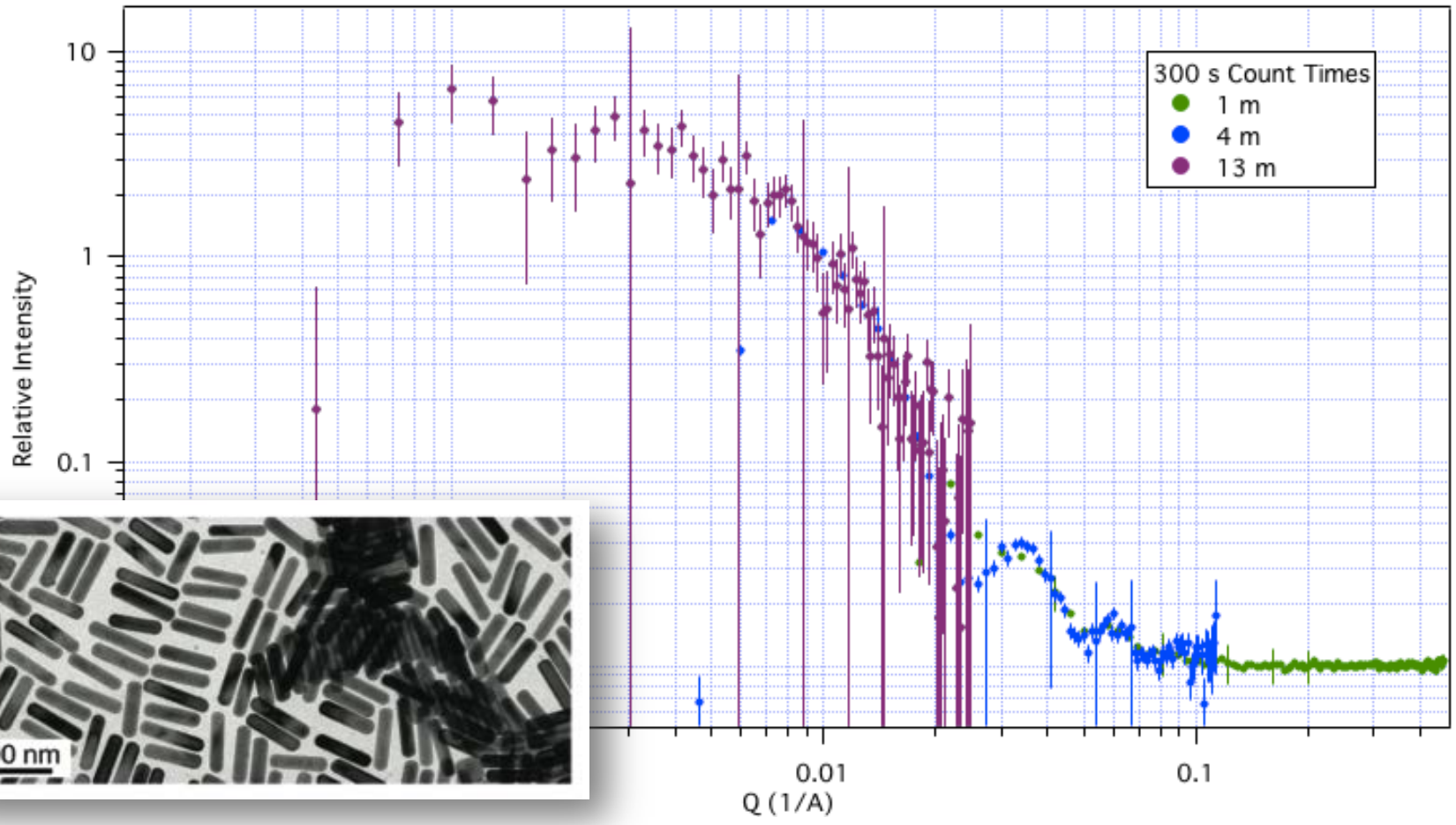

**So now we know!**

- **Detector distances, guides**
- **Time to count**
- **Sample thickness (1 mm) to use**
- **That our samples should work**
- **Approximately how many samples to prepare**
- **We can't use $H_2O$ as our solvent.**

**Great information to add to a beam time proposal!**
**Demonstrates the proposal is feasible.**

# A Real Example

**Au Nanorods are dilute typically. Will I see anything?**
**Volume fraction determined from UV-Vis (0.0004%)**




**We get scattering, but need to count longer.**

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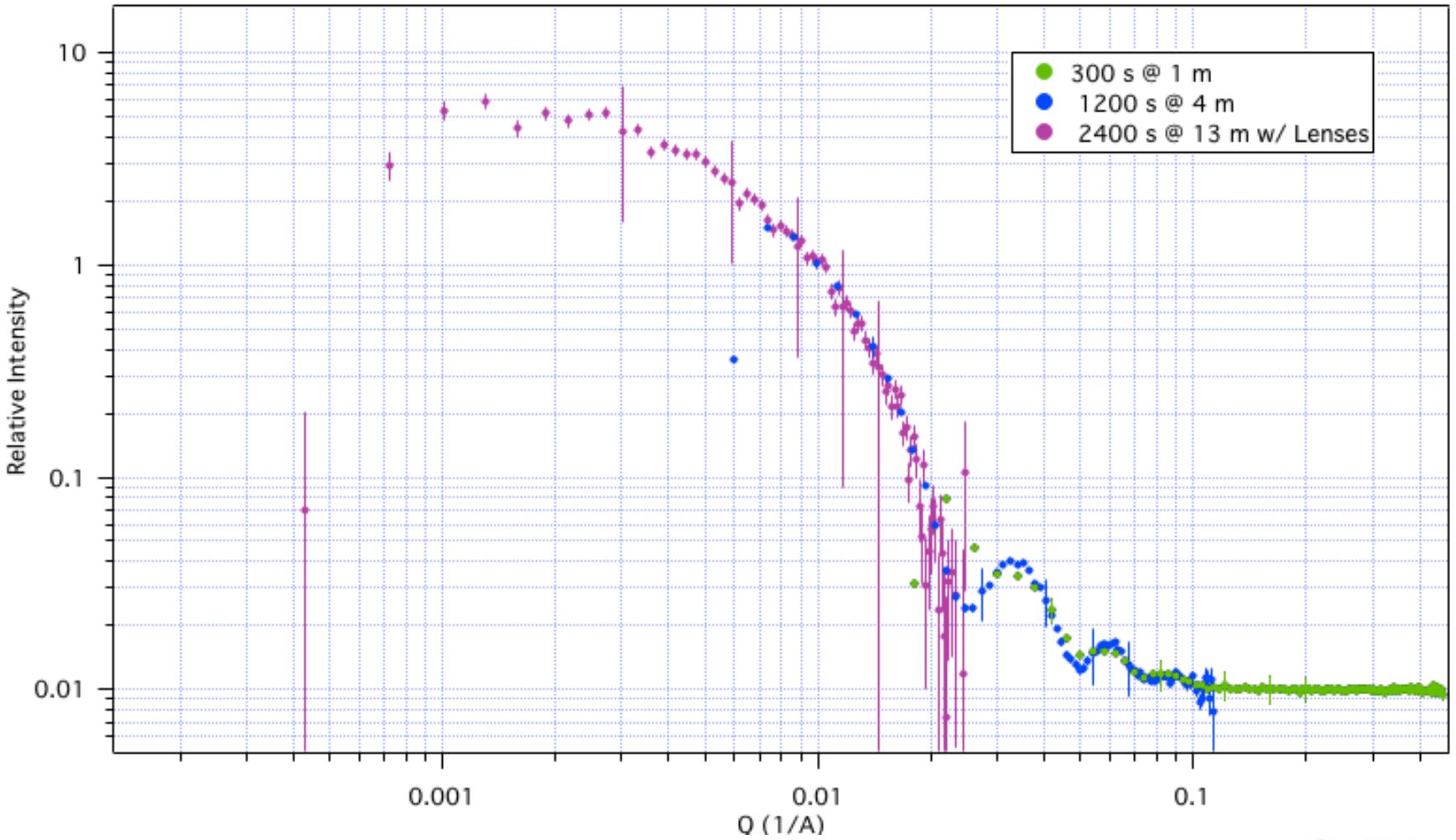
# A Real Example

**By selectively increasing count times, we get MUCH better data.**

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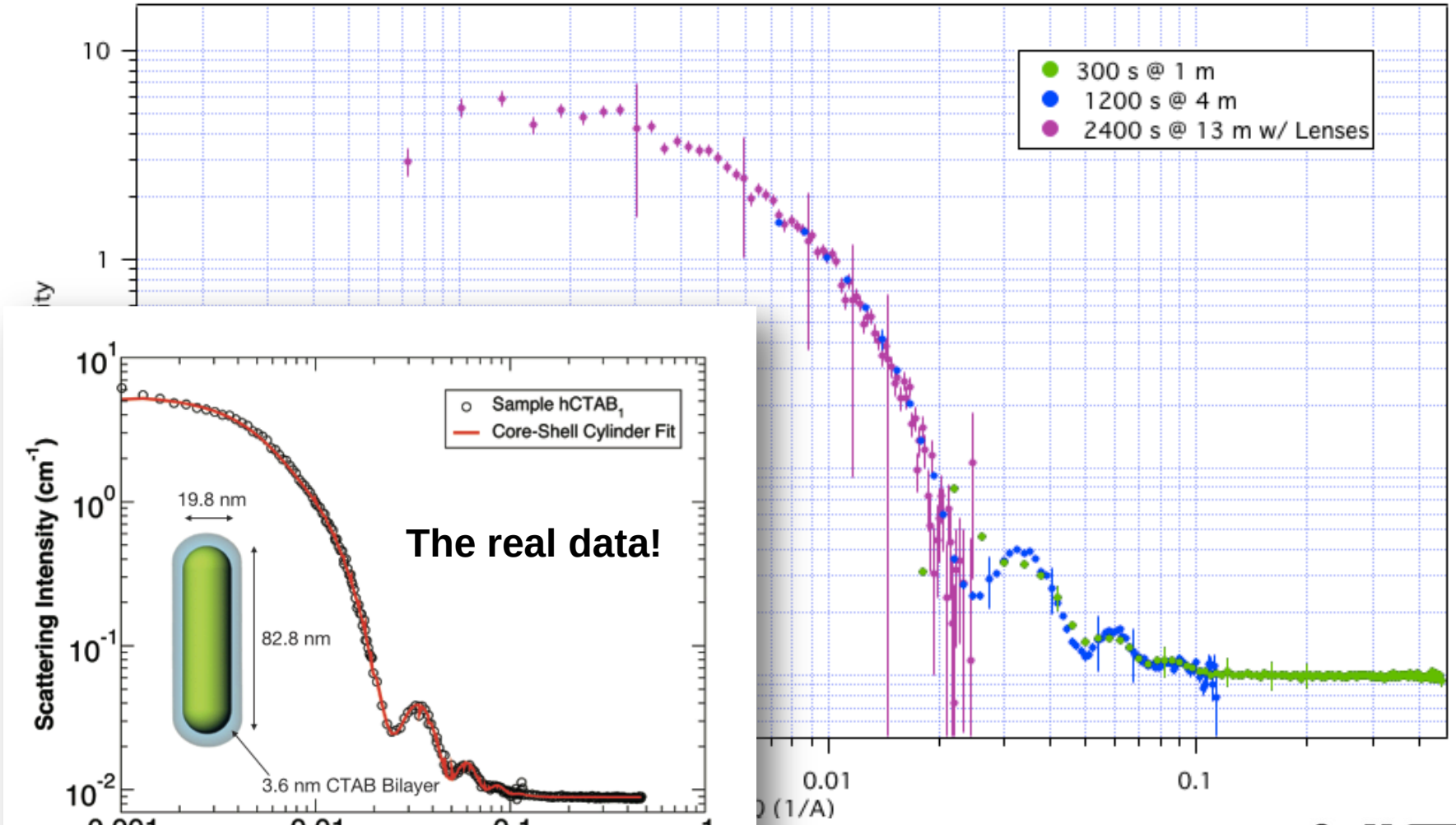
# A Real Example

**SASCALC is a great estimate for what we should expect to measure.**
**Doing USANS? Use UCALC.**







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# Other Tools on the NCNR Website

## http://www.ncnr.nist.gov/

| | |
|---|---|
| • SANS Homepage | /programs/sans |
| • **Calculation tools** | **/resources/index.html** |
| • Nuclear properties | /resources/n-lengths |
| • Manuals & Tutorials | /programs/sans/data/index.html |
| • **Reduction and Analysis** | **/programs/sans/data/red_anal.html** |
| • Video tutorials | /programs/sans/data/movies/reduction_analysis_movies.html |
| • Instrument information | /programs/sans/sans_inst.html |
| • Available Equipment | /programs/sans/equipment/index.html |
| • User Laboratories | /userlab |
| • Access information! | /access.html |
| • Proposal information | /beamtime.html |
| • **Monetary Assistance** | **/outreach.html (Support for first time users!)** |
| • Summer School notices | /summerschool |

| | |
|---|---|
| • **The SANS Toolbox** | **/staff/hammouda/the_SANS_toolbox.pdf (Almost everything you could need!)** |

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