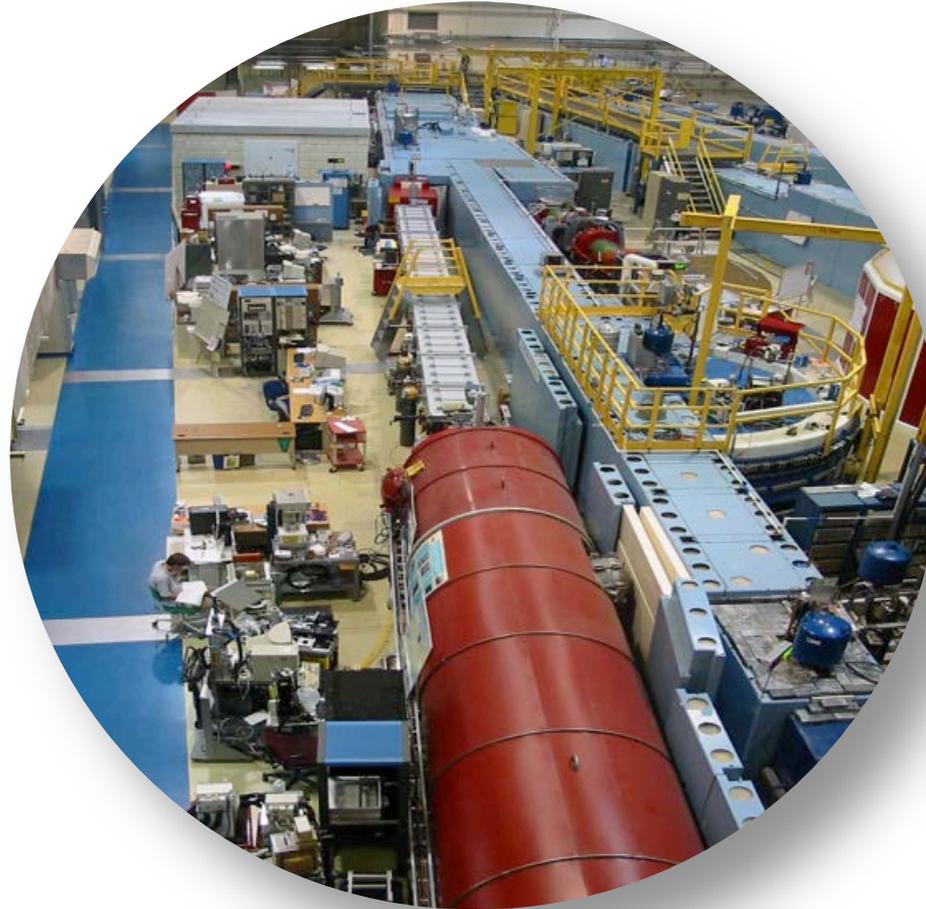


SANS and USANS Experiment Planning



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Case Western Reserve University
(former NCNR NRC postdoc)



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 ($\geq 99\%$ 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)

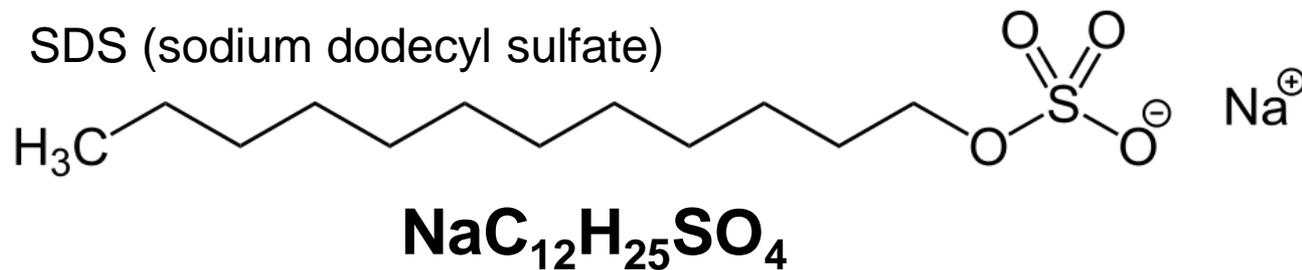
Scattering Length Density (SLD)

“Bound coherent scattering length”

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

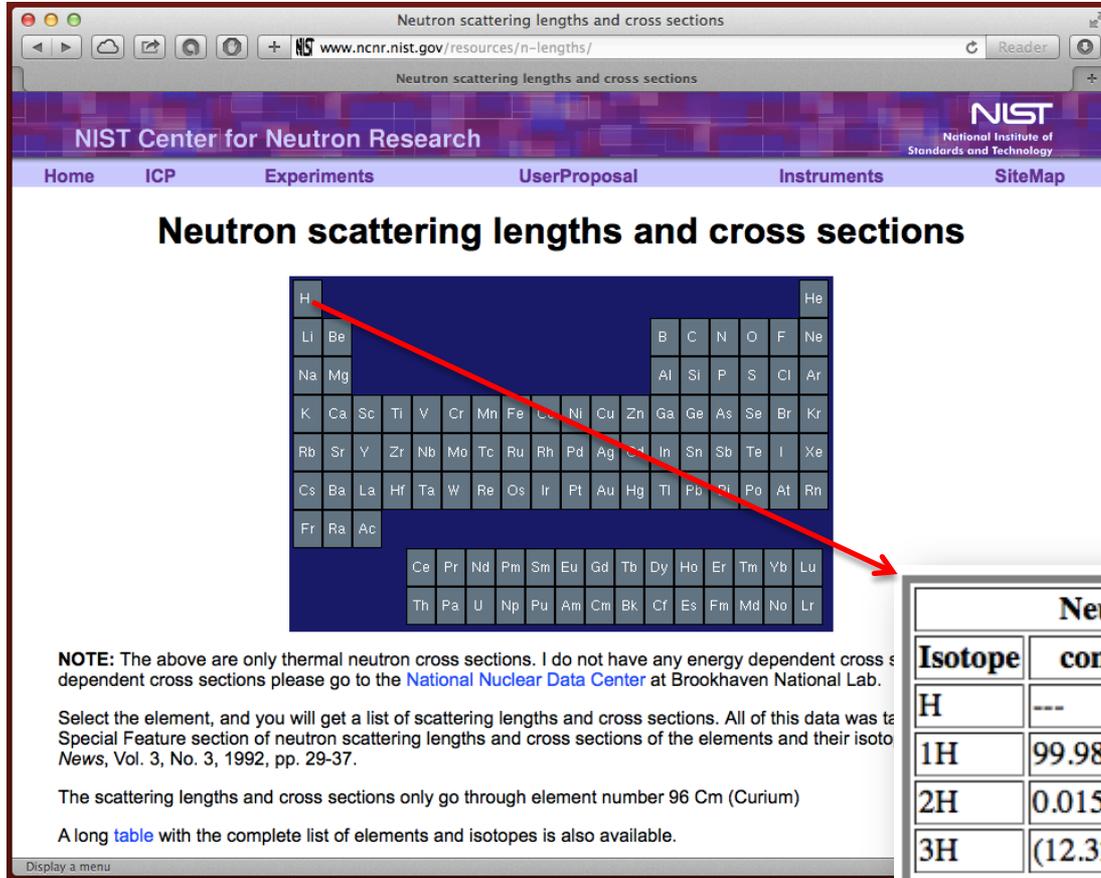
Usually given in units of inverse squared Angstrom or centimeter (\AA^{-2} or cm^{-2}).

So let's calculate the SLD of SDS:



Scattering Length Density – The Long Way

<http://www.ncnr.nist.gov/n-lengths>



The screenshot shows the NIST Center for Neutron Research website. The main heading is "Neutron scattering lengths and cross sections". Below it is a periodic table where the element Hydrogen (H) is highlighted. A red arrow points from the highlighted Hydrogen in the periodic table to a detailed data table. The data table is titled "Neutron scattering lengths and cross sections" and has columns for Isotope, conc, Coh b, Inc b, Coh xs, Inc xs, Scatt xs, and Abs xs. The value for the coherent scattering length (Coh b) of Hydrogen is -3.7406, which is circled in red. A red arrow also points from the equation $\rho = \frac{1}{V_m} \sum_{i=1}^n b_{c,i}$ to this circled value.

NOTE: The above are only thermal neutron cross sections. I do not have any energy dependent cross sections please go to the [National Nuclear Data Center](#) at Brookhaven National Lab.

Select the element, and you will get a list of scattering lengths and cross sections. All of this data was taken from the Special Feature section of neutron scattering lengths and cross sections of the elements and their isotopes, *Neutron News*, Vol. 3, No. 3, 1992, pp. 29-37.

The scattering lengths and cross sections only go through element number 96 Cm (Curium)

A [long table](#) with the complete list of elements and isotopes is also available.

Isotope	conc	Coh b	Inc b	Coh xs	Inc xs	Scatt xs	Abs xs
H	---	-3.7390	25.274	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

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

Scattering Length Density – The Long Way

<http://www.ncnr.nist.gov/n-lengths>

Neutron scattering lengths and cross sections							
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$$\rho = \frac{1}{V_m} \sum_{i=1}^n b_{c,i} \quad 1 \text{ fm} = 1 \text{ fermi} = 10^{-5} \text{ Angstrom}$$

$$\rho = \frac{1}{(474.28 \text{ \AA}^3)} \left\{ \begin{array}{cccccc} \text{Na} & & \text{C} & & \text{H} & & \text{S} & & \text{O} \\ 3.63 & + & 12(6.65) & + & 25(-3.74) & + & 2.80 & + & 4(5.80) \end{array} \right\} \text{ fm}$$

Volume of 1 SDS molecule calculated from mass density

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

Scattering Length Density – The Easy Way

<http://www.ncnr.nist.gov/resources/activation>

NIST Center for Neutron Research

[Home](#) [Instruments](#) [Science](#)

Material

NaC12H25SO4

Neutron Activation

For rabbit system

Thermal flux	Cd ratio	Thermal/fast ratio
1e8	0	0
Mass	Time on beam	Time off beam
1	10	1 y

Absorption and Scattering

Density	Thickness	<input type="button" value="Calculate"/>
1.01	1	
Source neutrons	Source X-rays	
6 Ang	Cu Ka	

Thickness

Units: cm

The material thickness in cm is used scattered incoherently. Leave it at

NaC12H25SO4 at 1.01 g/cm³

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/cm²/s for a 1e8 n/cm²/s beam.

$$= 3.37 \times 10^{-7} \text{ \AA}^{-2}$$

Scattering Length Density – The Easy Way

<http://www.ncnr.nist.gov/resources/activation>

D2O at 1.10 g/cm³

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/cm²/s for a 1e8 n/cm²/s beam.

NaC12H25SO4 at 1.01 g/cm³

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/cm²/s for a 1e8 n/cm²/s beam.

Estimating Scattering

Estimating Scattering in Igor Pro

For uniform ellipsoidal micelles in a solvent:

$$I(q) \propto \phi (\underbrace{\rho_{ell} - \rho_{solv}}_{\text{Difference in SLDs or the "Contrast"}})^2 \cancel{F(q)} + Bkg$$

Scattered Intensity

Volume Fraction

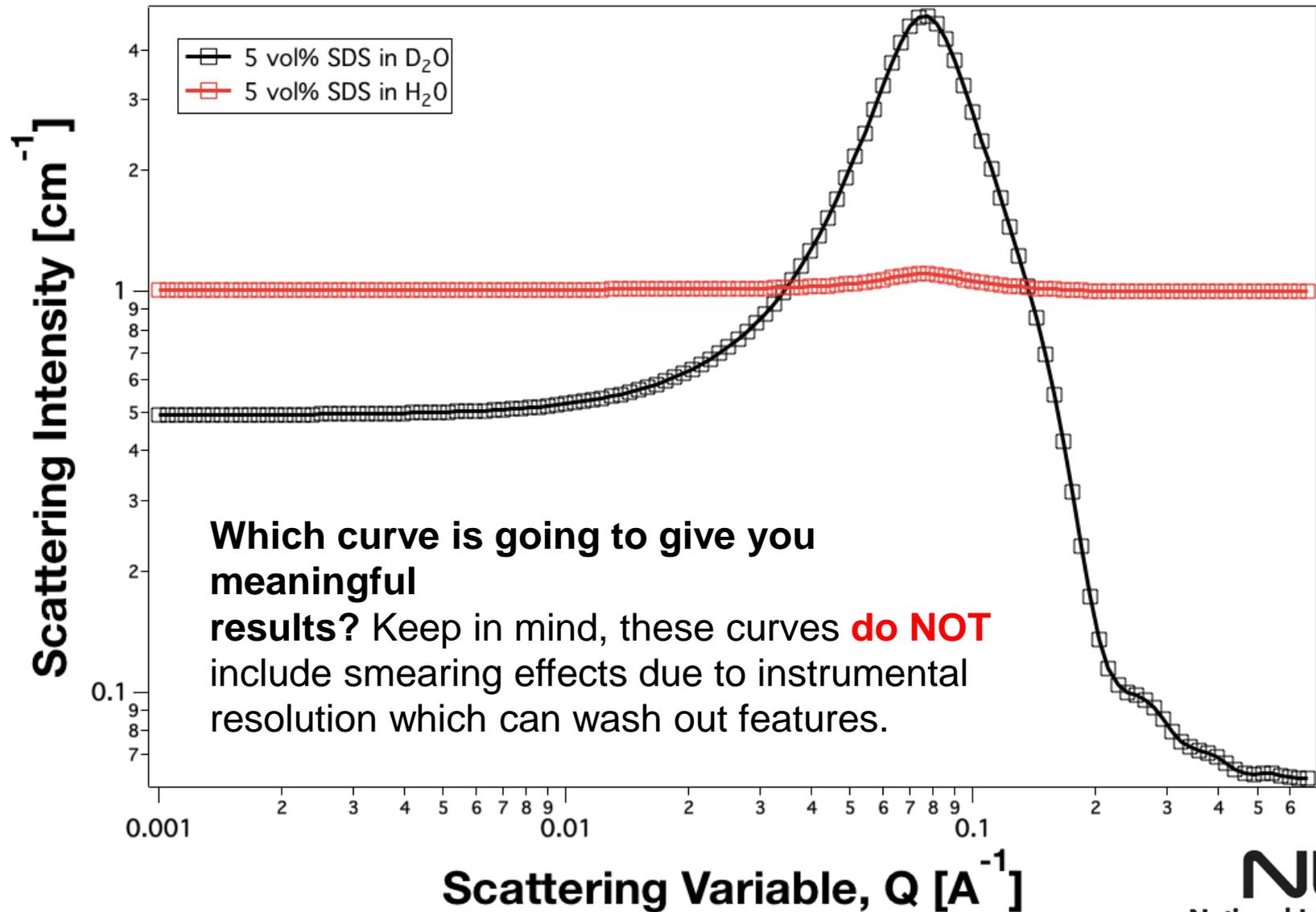
Incoherent Background
"noise" from Hydrogen (primarily)

Difference in SLDs
or the "Contrast"

What do we want for "good" data?

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

Estimating Scattering in Igor Pro

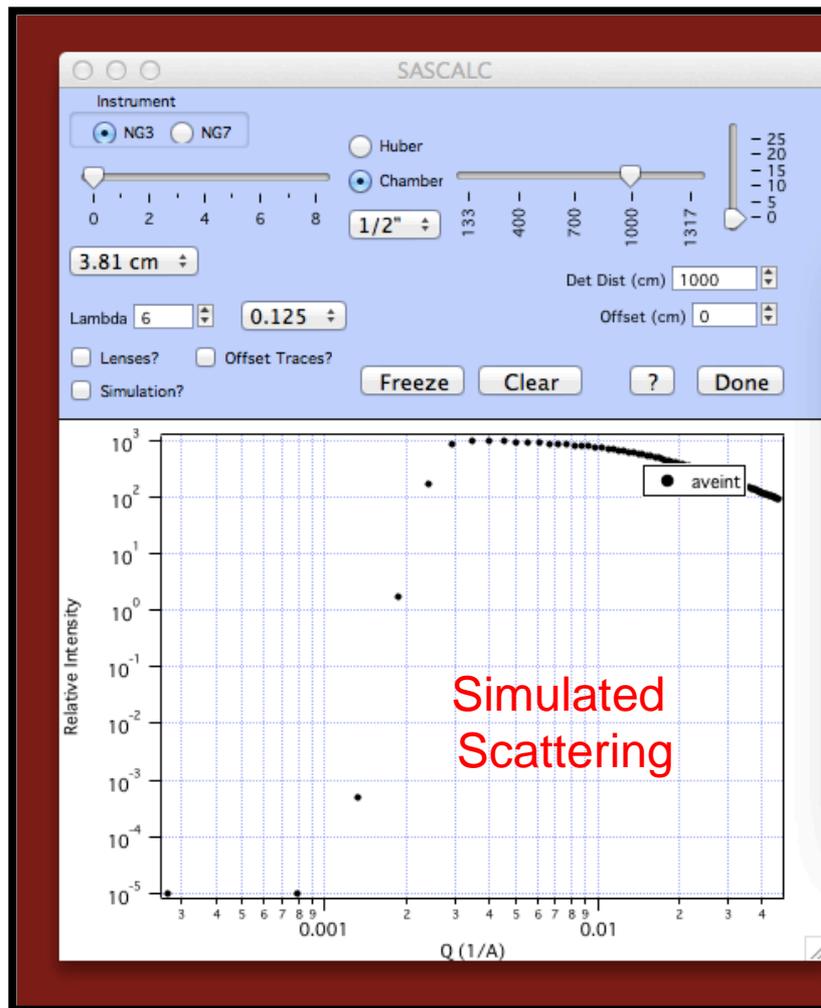


Instrument Configuration / SANS Simulation (SASCALC)

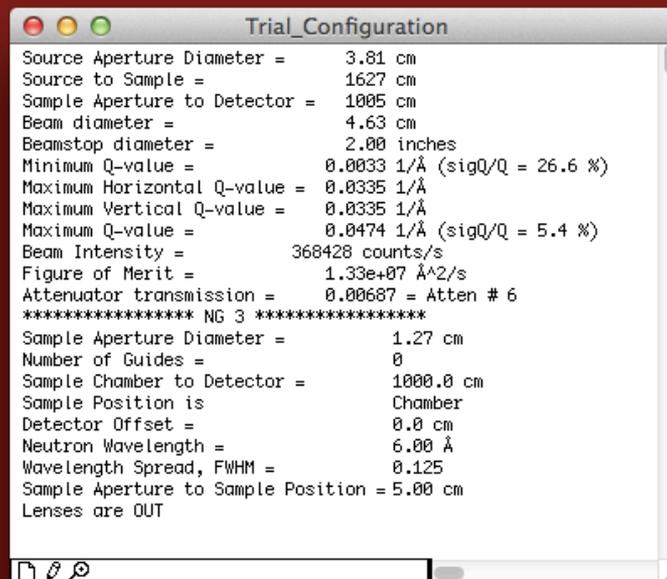
SASCALC (Inside Igor Pro Macros)

- 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)



Instrument Configuration



SASCALC (Inside Igor Pro Macros)

The screenshot shows the SASCALC software interface. The top section is a control panel with the following elements:

- Instrument:** Radio buttons for NG3 (selected) and NG7.
- Huber/Chamber:** Radio buttons for Huber and Chamber (selected).
- # of Guides:** A slider ranging from 0 to 8, currently set at 0.
- Wavelength:** A dropdown menu set to 1/2".
- Detector Distance (cm):** A slider ranging from 0 to 1317, currently set at 1000.
- Detector Offset (cm):** A vertical slider ranging from -25 to 0, currently set at 0.
- Lambda:** A dropdown menu set to 6.
- 0.125:** A dropdown menu.
- Buttons:** Lenses?, Offset Traces?, Simulation? (circled in red), Freeze, Clear, ?, Done.

The bottom section is a plot with the following characteristics:

- Y-axis:** Relative Intensity, logarithmic scale from 10⁻⁵ to 10³.
- X-axis:** Q (1/Å), logarithmic scale from 0.001 to 4.
- Data:** A series of points labeled 'aveint' showing a power-law decay.
- Label:** 'Wavelength' is written on the plot area.

of Guides

Detector Distance (cm)

Detector Offset (cm)

Use Focusing Lenses (13 m)?

Simulation?

Wavelength

SASCALC (Inside Igor Pro Macros)

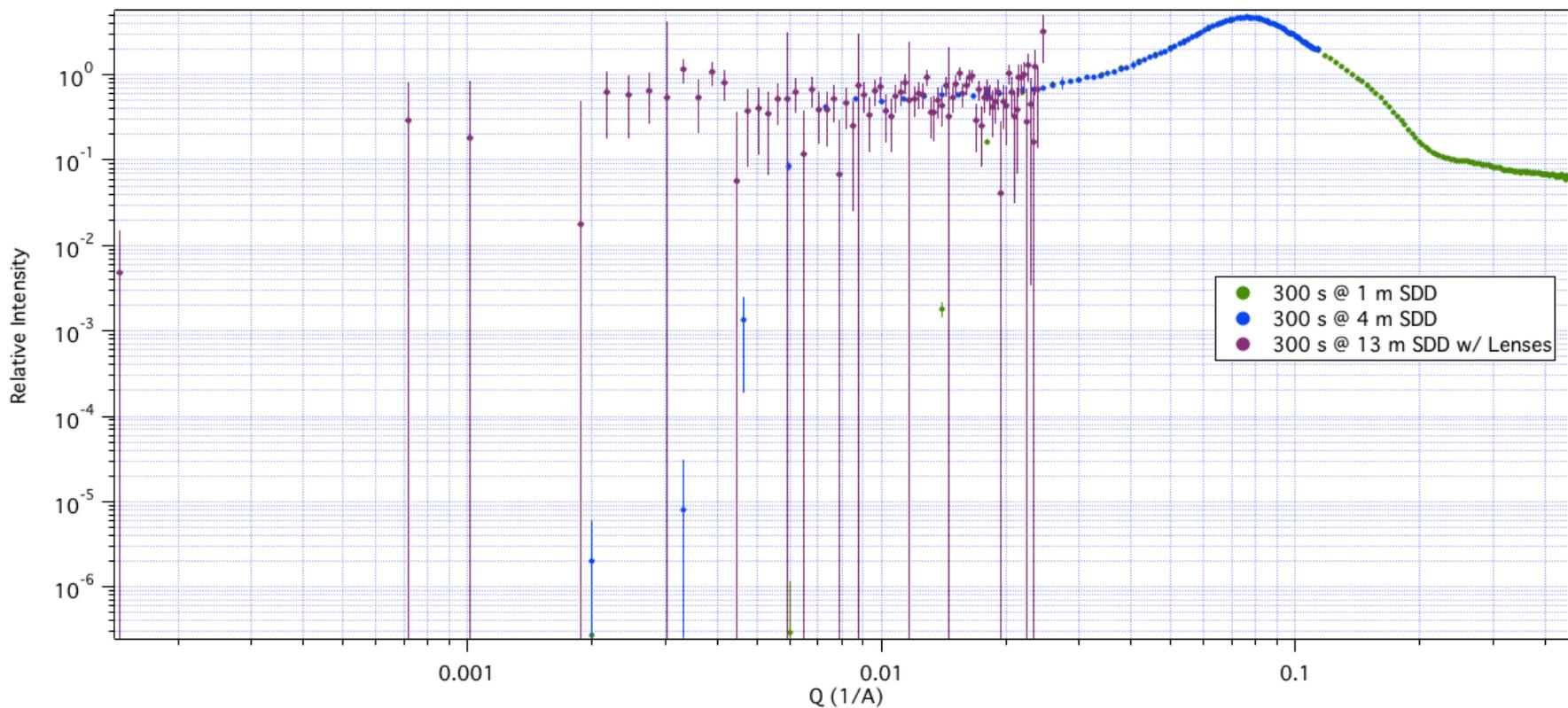
The screenshot displays the Igor Pro software interface with several windows open:

- SASCALC:** Instrument settings for NG3/NG7, Huber/Chamber, and various parameters like Source Aperture Diameter (3.81 cm), Lambda (6), and 0.125. Includes a plot of Relative Intensity vs. Q.
- Trial_Configuration:** Lists parameters such as Source Aperture Diameter (3.81 cm), Source to Sample (1627 cm), Sample Aperture to Detector (1005 cm), Beam diameter (4.63 cm), and Neutron Wavelength (6.00 Å).
- Curve Fit Setup:** Shows Data Set (Simulation), Function (Ellipsoid_SC), and Coefficients (coef_EOR_SC). Includes a table of parameters and fit statistics.
- 1D SANS Simulator:** Model Function (EllipsoidForm), Sample Setup (Counting time: 300, Thickness: 0.1, Sample Transmission: 0.8), and Simulation Results (Total detector counts: 0, Estimated count rate: 0, etc.).
- Graph0:** Plot of Intensity (cm⁻¹) vs. q (Å⁻¹) showing a peak at approximately q = 0.08.

parameters_EOR	coef_EOR_SC	Hold_EOR_SC	LoLim_EOR_SC	HiLim_EOR_SC	epsilon_EOR_SC
volume fraction	0.05	1			1.0001e-06
R(a) rotation ax	15	1			0.002
R(b) (A)	24	1			0.04
SLD ellipsoid (A)	3.37e-07	1			2e-10
SLD solvent (A ³)	6.38e-06	1			7.3e-10
charge	20	0			0.002
monovalent salt (F)	0	0			1e-10
Temperature (K)	298	0			0.0298
dielectric const	78	0			0.0078
incoh. bkg (cm ⁻¹)	0.06	0			1.0001e-06

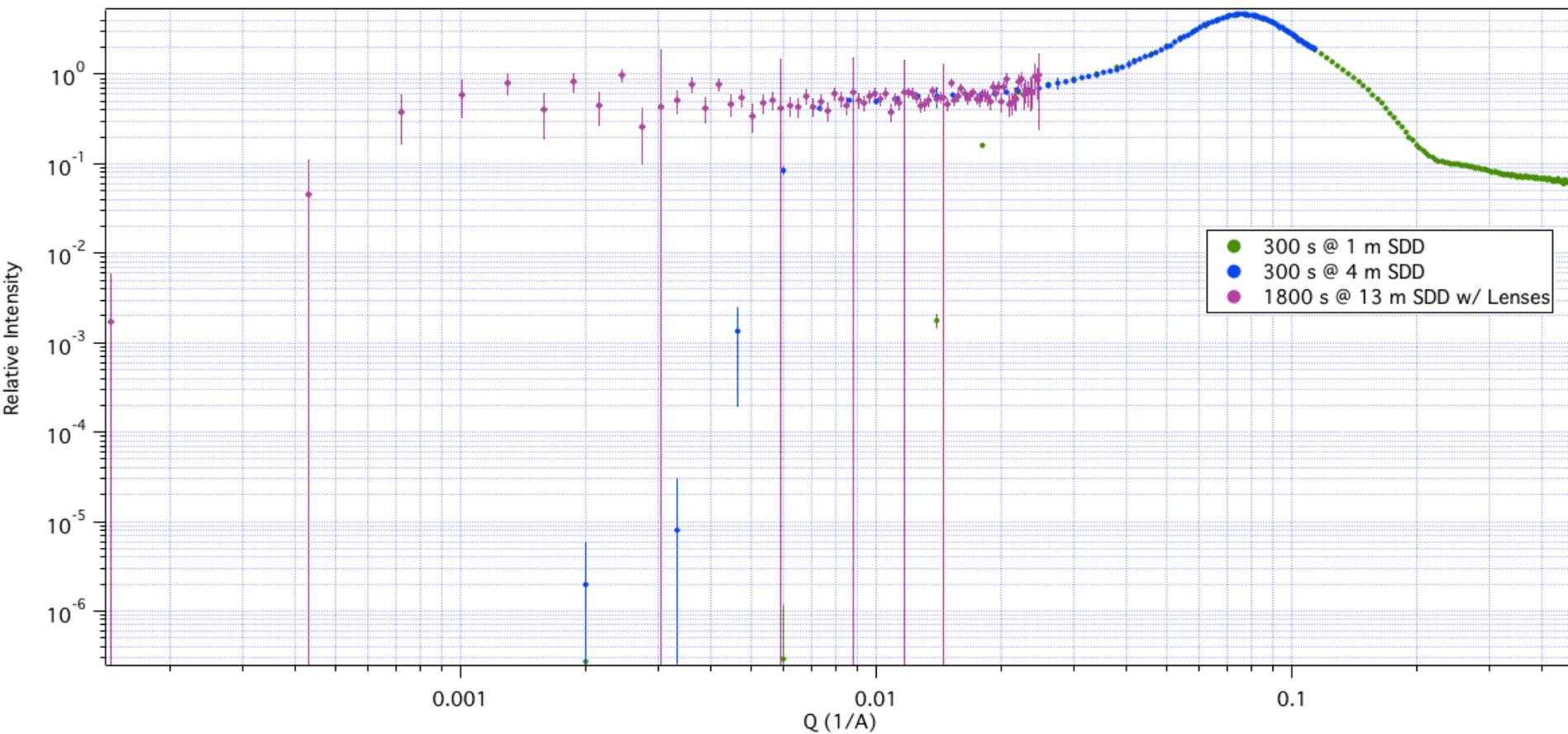
SASCALC (Inside Igor Pro Macros)

Counting for 300 s at each detector distance:



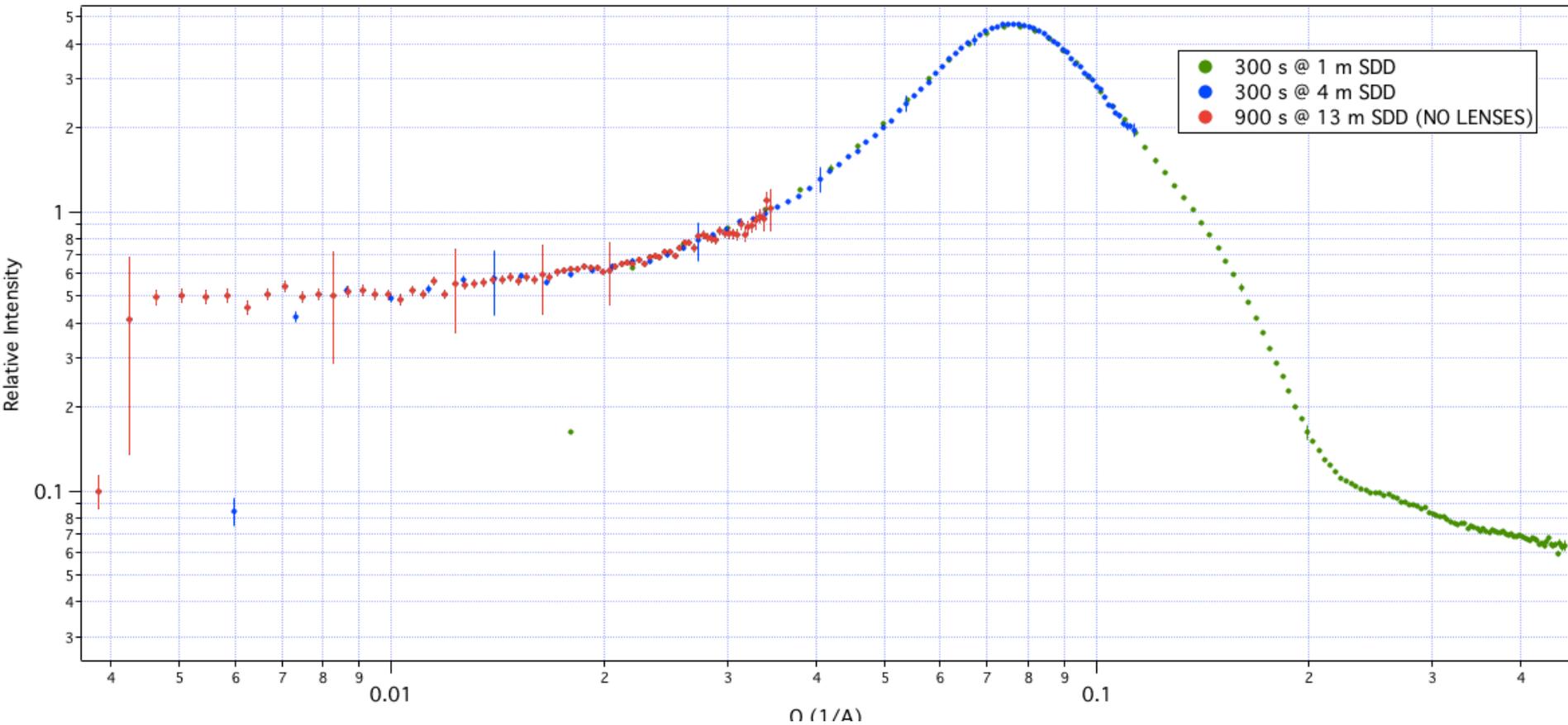
SASCALC (Inside Igor Pro Macros)

Counting for 1800 s at 13 m detector distance



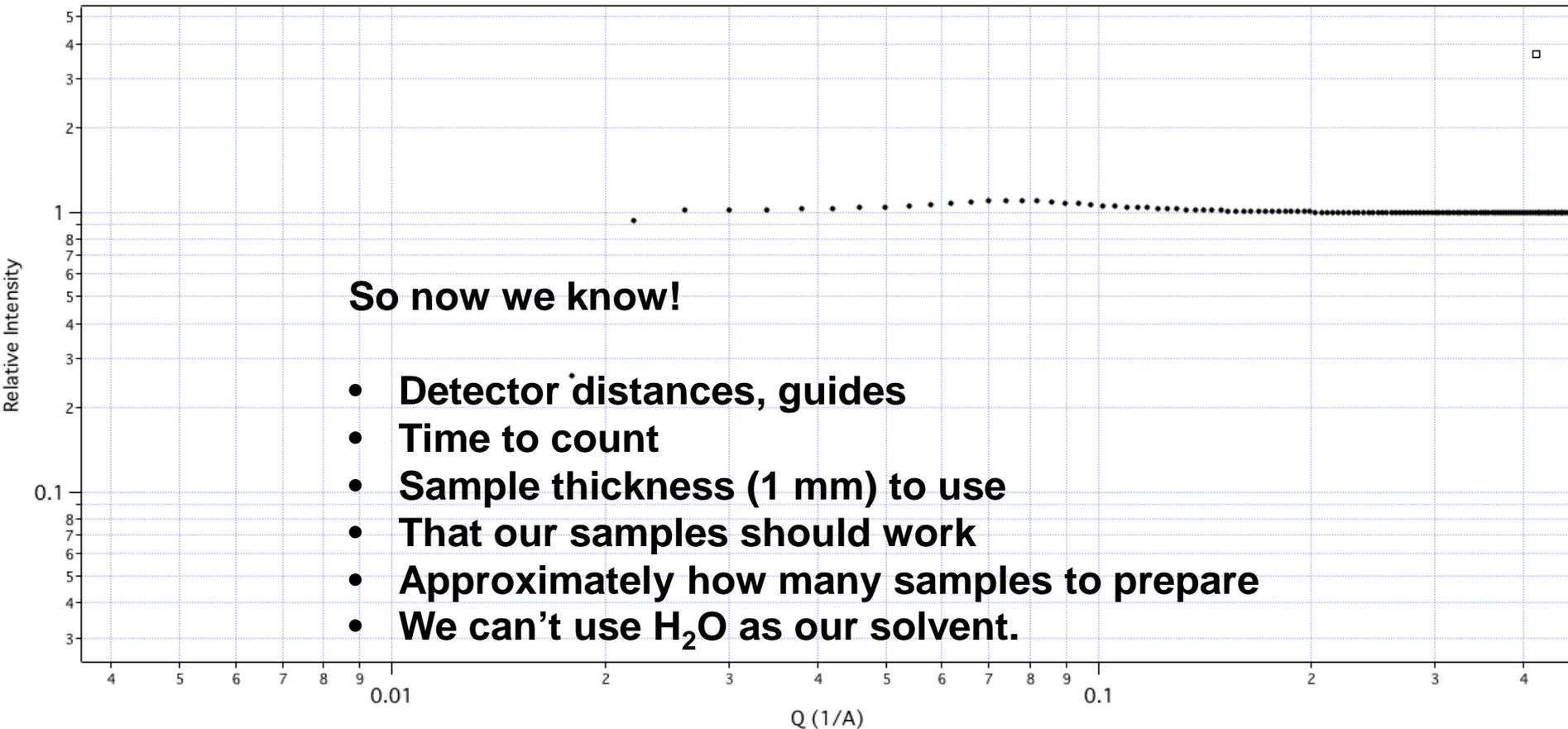
SASCALC (Inside Igor Pro Macros)

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



SASCALC (Inside Igor Pro Macros)

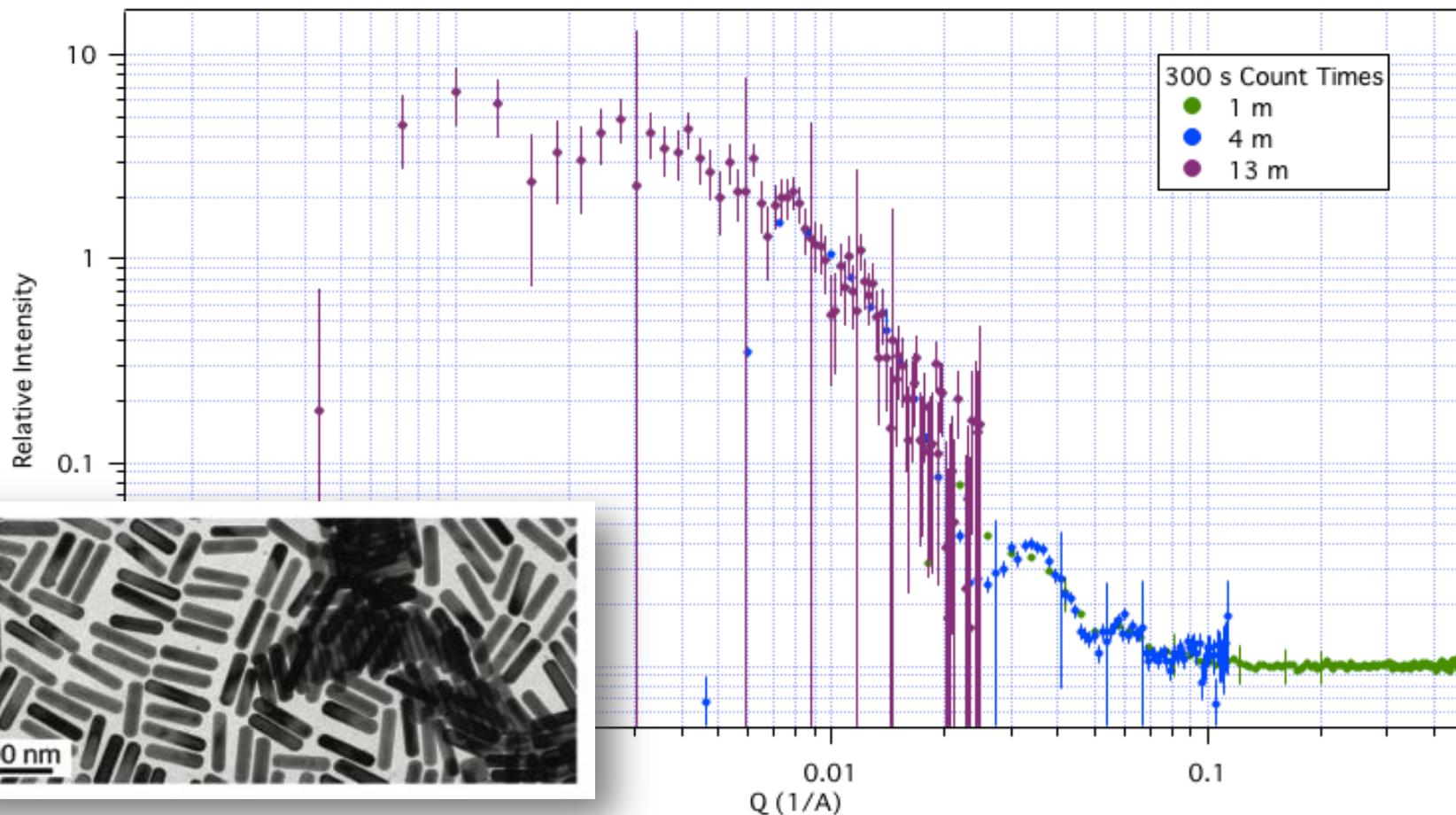
**Counting for 1 day at 1 m detector distance in H₂O – No signal essentially.
Waste of neutrons/time/money.**



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

A Real Example

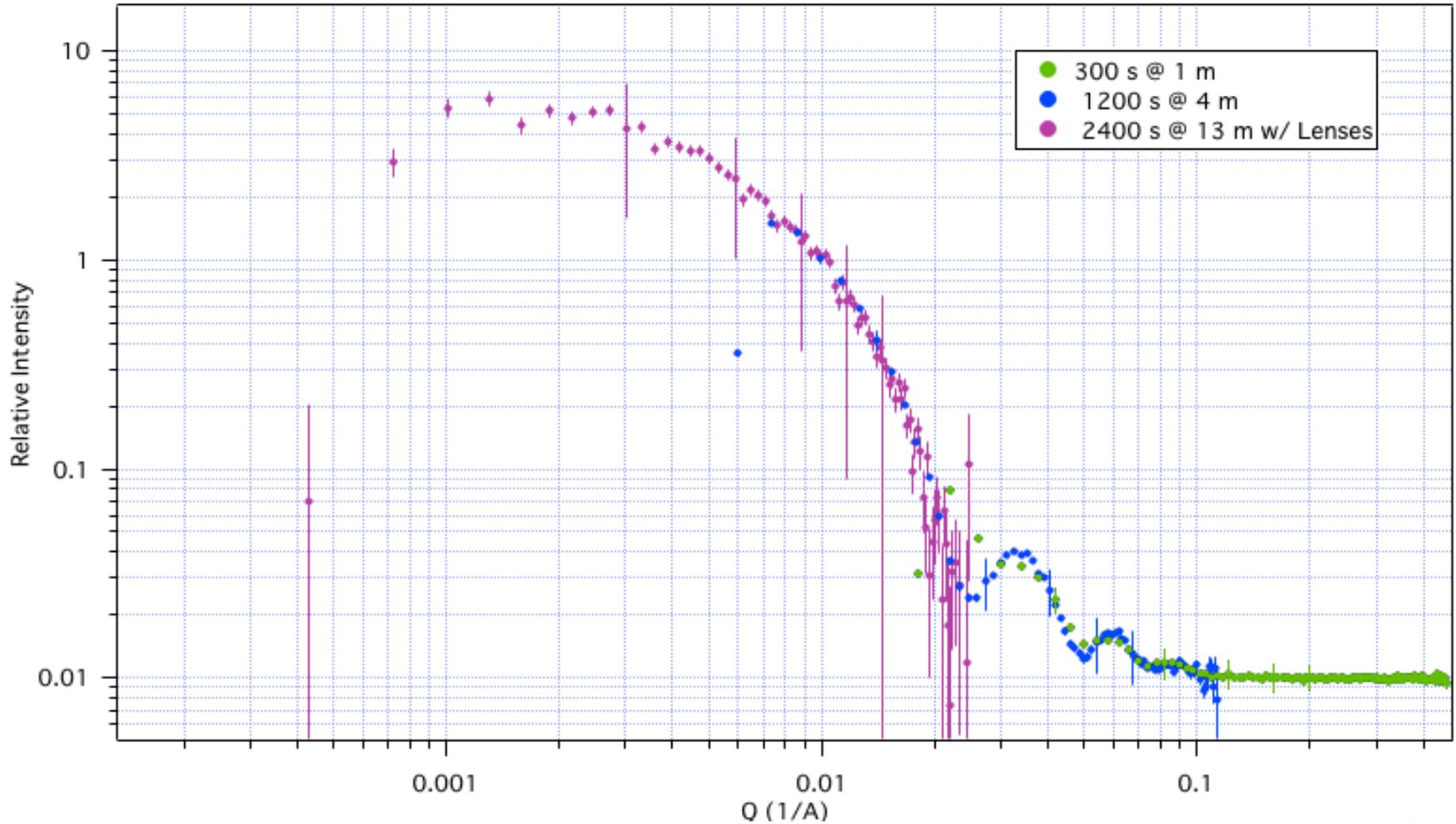
**Au Nanorods are dilute typically. Will I see anything?
Volume fraction determined from UV-Vis (0.0004%)**



We get scattering, but need to count longer.

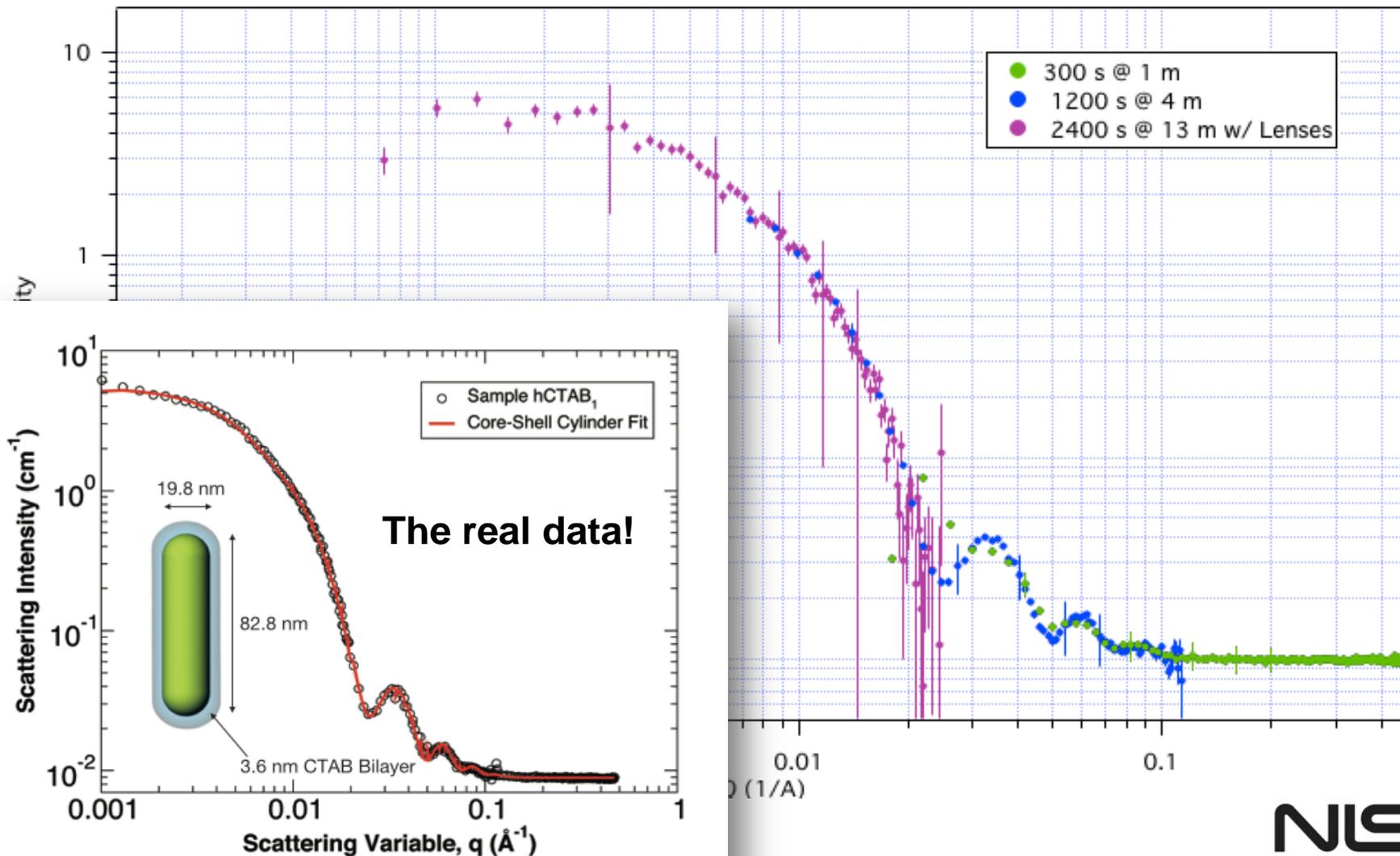
A Real Example

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



A Real Example

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



Other Tools on the NCNR Website

<http://www.ncnr.nist.gov/>

- SANS Homepage
 - **Calculation tools**
 - Nuclear properties
 - Manuals & Tutorials
 - **Reduction and Analysis**
 - Video tutorials
 - Instrument information
 - Available Equipment
 - User Laboratories
 - Access information!
 - Proposal information
 - **Monetary Assistance**
 - Summer School notices
- [/programs/sans
/resources/index.html](/programs/sans/resources/index.html)
- </resources/n-lengths>
- </programs/sans/data/index.html>
- [**/programs/sans/data/red_anal.html**](/programs/sans/data/red_anal.html)
- /programs/sans/data/movies/reduction_analysis_movies.html
- /programs/sans/sans_inst.html
- </programs/sans/equipment/index.html>
- </userlab>
- </access.html>
- </beamtime.html>
- [**/outreach.html \(Support for first time users!\)**](/outreach.html)
- </summerschool>
-
- [**/staff/hammouda/the_SANS_toolbox.pdf**](/staff/hammouda/the_SANS_toolbox.pdf)
(Almost everything you could need!)

• **The SANS Toolbox**