

# We CANS do it: would a SANS on PC-CANS be worth it?

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## Abstract

The proposed prototype Canadian Compact Accelerator-driven Neutron Source (PC-CANS) presents a cost-effective solution to address the shrinking global availability of neutron beams. Designed to support a range of applications, including Small Angle Neutron Scattering (SANS), neutron imaging, boron neutron capture therapy, and radioisotope production, PC-CANS aims to restore and enhance Canada's neutron science capabilities. Benchmarking against the LOQ instrument at the ISIS Neutron and Muon Source demonstrates that a PC-CANS SANS, despite operating with lower neutron flux, would provide comparable data quality for a variety of scientifically interesting samples with only modest increases in measurement duration. A set of well-characterized samples—including lipid bilayers for membrane structure and lipid domain monitoring, as well as scattering standards such as meso-porous silicalite and silver behenate—were measured on LOQ under both standard and reduced-flux configurations. The initial results show that with only an approximate sixfold increase in acquisition time, data was reproducible at a usable quality. This suggests that an SANS instrument at PC-CANS will be a valuable tool for a wide range of scientific fields, from material science to biophysics. With ongoing improvements, ranging from technological advances to AI-driven data collection, PC-CANS has the potential to become a key resource for Canadian researchers and further foster international scientific collaboration.

**Key words:** small angle neutron scattering, SANS, CANS, neutron instrumentation, lipids

## 1. Introduction—national context

For technical, regulatory, and financial reasons, the global availability of neutron beams is diminishing. Countries, like Canada, with a proud tradition of neutron scattering are therefore increasingly focused on innovative means to maintain and expand access to neutron beams for their research base. Canada, home to the highly regarded Chalk River Nuclear Laboratories (now Canadian Nuclear Laboratories), played a key role in producing the country's second Nobel Laureate in Physics, Bertram Brockhouse. Presently, Canada faces operational challenges that have led to various program cuts and intermittent shutdowns over the years, with the final shutdown of the NRU reactor occurring on 31 March 2018 [1].

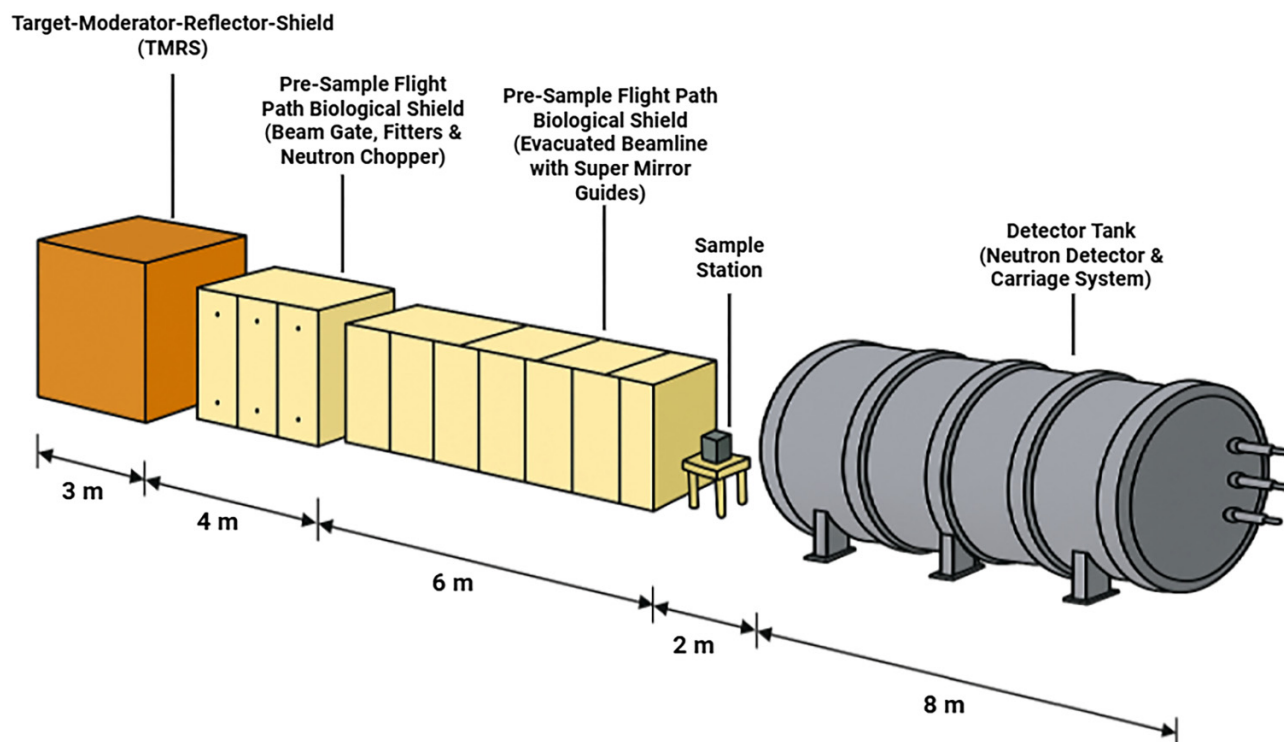
Financial challenges have hindered Canada's potential as a global leader in neutron production and science. With a globally shrinking supply of neutrons and the NIMBY (Not In My Backyard) perception surrounding research reactors, compact accelerator-driven neutron sources (CANS) are emerging as an attractive solution. CANS offer the potential for an intense, pulsed neutron source at a significantly lower capital cost compared to conventional spallation or fission reactor sources, while also facing much less public stigma. The pro-

posed prototype Canadian CANS (PC-CANS) represents a crucial step towards rebuilding Canada's neutron capabilities in this evolving technological landscape [2–5].

The proposed PC-CANS is a collaborative pan-Canadian initiative designed to support a range of applications. The PC-CANS will serve two neutron science instruments: small angle neutron scattering (SANS) and neutron imaging, along with a boron neutron capture therapy (BNCT) station and a beamline for fluorine-18 radioisotope production for use in positron emission tomography in the host region. To meet the diverse demands of these applications, the system will employ a linear accelerator (linac) capable of delivering 10 MeV protons with a peak current of 20 mA at a 5% duty cycle (10 kW). The linac will utilize a Radio Frequency Quadrupole and Drift Tube Linac (DTL) configuration, complemented by a post-DTL pulsed kicker system, to simultaneously direct macro-pulses to each of the end-stations [6–8]. The neutron production targets, made from beryllium, will be specifically engineered to handle the high beam intensity required for both neutron science and BNCT applications [2, 4].

A computational study of the PC-CANS design, particularly its SANS capability, has shown no significant technical barriers. The conceptual SANS instrument has a primary

**Fig. 1.** Simplified schematic layout of the proposed prototype Canadian Compact Accelerator-driven Neutron Source small angle neutron scattering instrument.



(moderator-sample) flightpath of around 13 m and a variable secondary (sample-detector) flightpath between 2 and 8 m with a movable 1 m<sup>2</sup> detector in an evacuated tank, as depicted in Fig. 1. It is anticipated the beam on sample will be routinely collimated to 10 mm diameter. Under typical Stage 1 PC-CANS operating conditions, with 2 kW time-averaged proton beam power directed at the SANS target, calculations suggest the time-average flux of neutrons at the sample will be approximately a factor six lower than that of the LOQ instrument at the ISIS First Target Station (2 kW at 800 MeV), a first-generation, fixed geometry TOF-SANS, which has supported a large and scientifically diverse user community for over 35 years [9].

Despite this difference, given that many measurements at the LOQ instrument require only 10–30 min of data collection time, the necessarily longer collection time for the PC-CANS SANS instrument is not expected to pose a limitation for many static samples, such as those studied in hard condensed matter or polymer science. Furthermore, the PC-CANS target is expected to evolve, eventually handling up to 10 kW of linac power (Stage 3), which will increase its flux and make it competitive with the LOQ instrument in terms of performance. However, this leaves a question mark about the practical usability of an instrument with such a low flux to begin with. Through comparison of repeat measurements on representative samples undertaken at representative instrument flux settings, this paper will conclusively demonstrate that scientifically usable data can be obtained at the lower flux levels projected for the early stages of operation of the PC-CANS SANS.

### 1.1. PC-CANS SANS

To assess the anticipated scientific capabilities of the proposed SANS instrument, we conduct benchmarking against similar instruments at other pulsed CANS facilities, as well as an established SANS instrument at a medium-brightness pulsed spallation source, specifically the LOQ instrument at the ISIS First Target Station [9].

For primary theoretical benchmarking, we chose the NOVA ERA reference design due to its advanced CANS technology, extensive data availability, and robust simulation methodologies [10]. Review of existing SANS instruments at the Low Energy Neutron Source (LENS) and Compact Pulsed Hadron Source (CPHS) shows performance levels comparable to NOVA ERA [11, 12]. LENS operates at 4 kW, producing a neutron flux of  $\approx 1 \times 10^4$  n/(cm<sup>2</sup>·s) with  $Q_{\min} = 0.008$  Å, while CPHS (16 kW at 2.5% duty cycle) targets  $\approx 1 \times 10^4$  n/(cm<sup>2</sup>·s) with  $Q_{\min} = 0.007$  Å. The interpolated data from NOVA ERA suggest a flux of  $\approx 1.2 \times 10^4$  n/(cm<sup>2</sup>·s) at  $Q_{\min} = 0.008$  Å with just 0.4 kW of accelerator power at 4% duty cycle—demonstrating significant advances in CANS [10]. Additionally, a key factor to consider is the proposed usage of a 20 K cold-finger moderator made of mesitylene, which will produce cold neutrons for the proposed PC-CANS. Both the NOVA ERA and PC-CANS designs retain neutrons above 2 Å.

In the PC-CANS Conceptual Design Report, we examine two repetition rate strategies [6]. Here, we focus on the strategy that is simpler and provides a more conservative estimate of flux at the sample. The approach fixes the duty factor of the proton beam at 5%, thus matching the duty cycle of the proton linac. As a result of this duty factor, there is a >30 ms

**Table 1.** Collimation and performance of the proposed small angle neutron scattering (SANS) instrument for the prototype Canadian Compact Accelerator-driven Neutron Source using a fixed duty factor at 5%, resulting in a beam power of 2 kW for Stage 1 and 10 kW for Stage 3.

Collimation (m)	Sample Detector (m)	Aperture 1 diameter (mm)	Aperture 2 diameter (mm)	$\lambda$ band (Å)	$Q_{\min}$ (Å <sup>-1</sup> )	$Q_{\max}$ (Å <sup>-1</sup> )	Flux at sample $n \text{ cm}^{-2}\text{s}^{-1}$	
							Stage 1	Stage 3
1	1	20	10	2-10.0	0.019	1.44	$2.2 \times 10^5$	$1.1 \times 10^6$
2	2	20	10	2-9.5	0.01	0.77	$1.2 \times 10^5$	$6.2 \times 10^5$
4	4	<b>20</b>	<b>10</b>	<b>2-8.3</b>	<b>0.0057</b>	<b>0.39</b>	<b><math>3.1 \times 10^4</math></b>	<b><math>1.5 \times 10^5</math></b>
6	6	20	10	2-7.4	0.0042	0.26	$1.4 \times 10^4$	$6.8 \times 10^4$
10	10	20	10	2-6.5	0.0029	0.16	$4.8 \times 10^3$	$2.4 \times 10^4$

Note: The bolded text represents the performance closest to the configuration of LOQ.\*

\*The LOQ  $Q_{\min} = 0.006 \text{ Å}^{-1}$ ,  $Q_{\max} = 0.24 \text{ Å}^{-1}$  on the main detector.

gap between proton pulses, creating dark times on the detector, where no neutrons are hitting the detector. As a result, the dark times are between 5 ms (1 m sample-to-detector distance) and 9.5 ms (10 m sample-to-detector distance). The corresponding beam frequency ranges from 27.5 to 30 Hz. For comparison, the High Brilliance Neutron Source (HBS) proposes a wavelength resolution of 5% with a repetition rate of 24 Hz [13]. Table 1 outlines the performance using the 5% duty factor configuration.

The SANS at the PC-CANS in Stage 1 operations (4 mA, 10 MeV, 5% duty factor) will produce an expected performance a factor of  $\approx 7$  less compared to LOQ in neutrons at the sample. Without consideration of instrumental improvements, our Stage 3 operations (20 mA, 10 MeV, 5% duty factor), which will be five times brighter than Stage 1, will be quite comparable to the performance of LOQ.<sup>1</sup> Further specifications in regards to the proposed PC-CANS design have been published elsewhere [2, 3, 6].

## 2. Methods and materials

The synthetic lipids 1,2-dipalmitoyl-sn-glycero-3-phosphocholine [di-16:0 PC, DPPC], 1,2-dipalmitoyl-d62-sn-glycero-3-phosphocholine [di-16:0 PC-d62, DPPC], 1,2-dioleoyl-sn-glycero-3-phosphocholine [18:1/18:1 PC, DOPC], and 1-palmitoyl-2-oleoyl-glycero-3-phosphocholine [16:0/18:1 PC, POPC] were purchased from Avanti Polar Lipids (Alabaster, AL). Cholesterol (Chol) was purchased from Sigma-Aldrich (St. Louis, MO). Silver Behenate was purchased from Thermo Fisher Scientific (Mississauga, Canada). Large-pore mesostructured silicalite (MSU-H) was purchased from Merck (Gillingham, UK).

Lipid samples were prepared by dissolving the lipids in HPLC grade chloroform (Sigma-Aldrich) to the desired concentration. A stream of argon gas was used to evaporate the solvent, and the samples were dried in a vacuum oven overnight. For bilayer structure experiments the samples were rehydrated with pure D<sub>2</sub>O, while for the domains experiments a 31% D<sub>2</sub>O solution was used to attain the desired contrast. Samples were hydrated to the desired concentrations (between 5 and 20 mg/mL). Following rehydration, lipid films were incubated for 30 min, followed by being subjected to

5 freeze-thaw-vortex cycles to disrupt multilamellarity. The samples were then extruded using a hand-held mini-extruder (Avanti Polar Lipids) through a 100 nm pore-diameter. The sample size distribution was confirmed to be monodisperse using dynamic light scattering. Samples were then loaded into 2 mm path-length quartz cuvettes (Hellma/Starna Scientific, UK). The silicalite and silver behenate powder samples were also loaded into the 2 mm path-length cuvettes, prior to measurement.

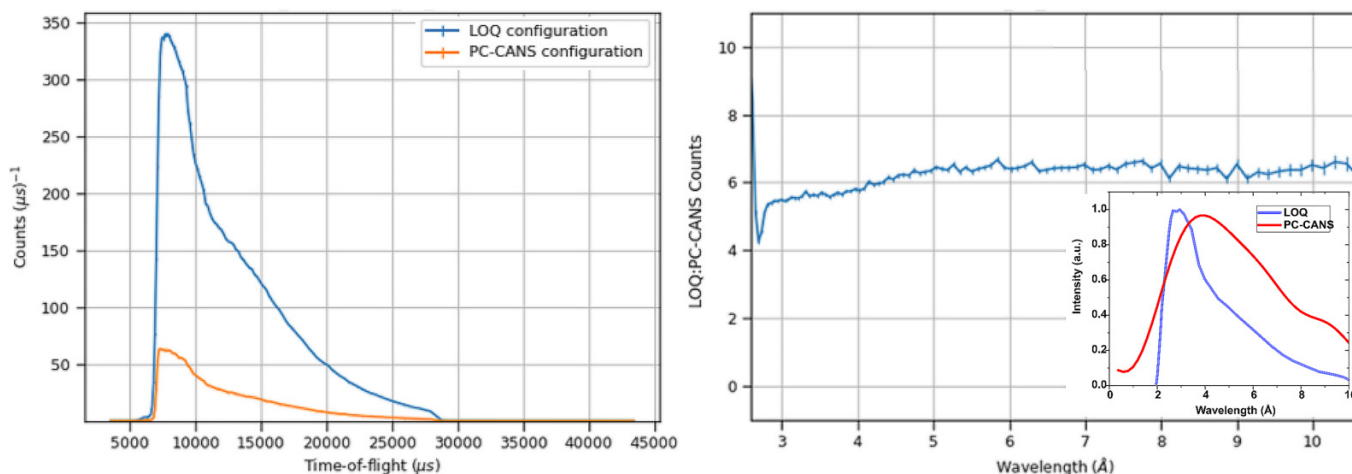
Raw scattering data were corrected for the incident neutron wavelength distribution, the detector efficiency and spatial linearity, the measured sample transmission, and the volume of sample illuminated, before being radially averaged and converted into the coherent elastic differential scattering cross-section,  $\frac{\partial \Sigma}{\partial \Omega}(Q)$ , hereafter simply intensity  $I$ , as a function of the scattering vector  $Q$ , using the Mantid framework (<https://mantidproject.org/>) [14]. Any contribution from instrumental and sample background scattering was removed by subtracting similarly processed data from an empty cuvette or cuvette containing pure solvent.

### 2.1. LOQ setup

For neutron scattering, the intensity and wavelength distribution of the neutron flux are critical factors that influence the quality of the scattering data, such as  $Q$ -range, resolution, and the signal-to-noise ratio of measurements. To validate the projected performance of the proposed PC-CANS SANS instrument, the measurement of samples on an operational instrument with a comparable flux were desired. In this regard we were fortunate to be granted the opportunity to use LOQ. LOQ is a pinhole-collimated SANS instrument with three upstream apertures, the diameters of which can be independently varied to suit the measurement requirements of a given sample. For the purposes of this study the second aperture was removed. The third (or sample) aperture, situated a few mm in front of the sample, along with the sample thickness, defines the illuminated volume. Changing the size of the first (or source) aperture is an effective way of changing the flux on the sample, albeit at the expense of a modest change in the instrument  $Q$ -resolution (eq. 5 from Mildner et al.) [15]. The flux change is proportional to the area of the aperture and so by reducing the diameter of the aperture from the usual 20 to 8 mm, the neutron flux was decreased by a factor of approximately 6.2, as seen in Fig. 2. This

<sup>1</sup> True for LOQ before the 2023 Target Station 1 upgrade.

**Fig. 2.** Two representations of the attenuation of the LOQ neutron flux by modifying Aperture 1. (Left) Neutron time-of-flight distributions normalized for integrated proton charge. (Right) LOQ : prototype Canadian Compact Accelerator-driven Neutron Source (PC-CANS) flux ratio as a function of neutron wavelength. Inset: comparison of the relative cold neutron spectra at the surface of the PC-CANS mesitylene moderator (red) and at the second LOQ beam monitor (blue). The data has been scaled for viewing ease. PC-CANS spectra was developed in ref. [6] and visualized using McTal (<https://iffgit.fz-juelich.de/zakalek/mctal>).



adjustment enabled a comparison of data quality between the LOQ configuration (Aperture 1 = 20 mm and Aperture 3 = 5 mm) compared to the projected Stage 1 PC-CANS configuration (Aperture 1 = 8 mm and Aperture 3 = 5 mm). Moreover, LOQ is a compact instrument with a moderator-sample distance of 11 m, of which 4 m is collimation, and a sample-main detector distance also of 4 m. This corresponds to one of the PC-CANS SANS configurations that has been modeled (see Table 1 highlight).<sup>2</sup>

### 3. Results and discussion

A variety of benchmarking samples were measured on LOQ to scope their measurement feasibility on the proposed PC-CANS SANS instrument. These included: standard calibration samples (eg, partially-deuterated polymer blends, silver behenate), hard matter samples (eg, polycrystalline porous silicalite), and biological soft matter samples (e.g., phospholipid vesicles, including contrast matching). Some of these samples also exhibited scattering patterns with structural features adding a resolution component to the exercise.

#### 3.1. Meso-porous silicalite

This material has been used in neutron scattering schools as it generates a feature-rich scattering pattern that can be suppressed by filling the mesopores with a contrast matching fluid. Being a polycrystalline powder it is also quite a strong scatterer. This sample was measured at three different Aperture 1 diameters: 20 mm (the normal setting on LOQ), 8 mm (producing a factor 6 reduction in flux to emulate the PC-CANS SANS), and 4 mm (producing a factor 25 reduction in flux). The reduced data are shown in Fig. 3. The data for the LOQ configuration were measured for 30  $\mu$ AHr ( $\sim$ 30 min),

<sup>2</sup>The adjustment of aperture 3 to 5 mm compensates for the increase in neutrons on sample from the Target Station 1 upgrade.

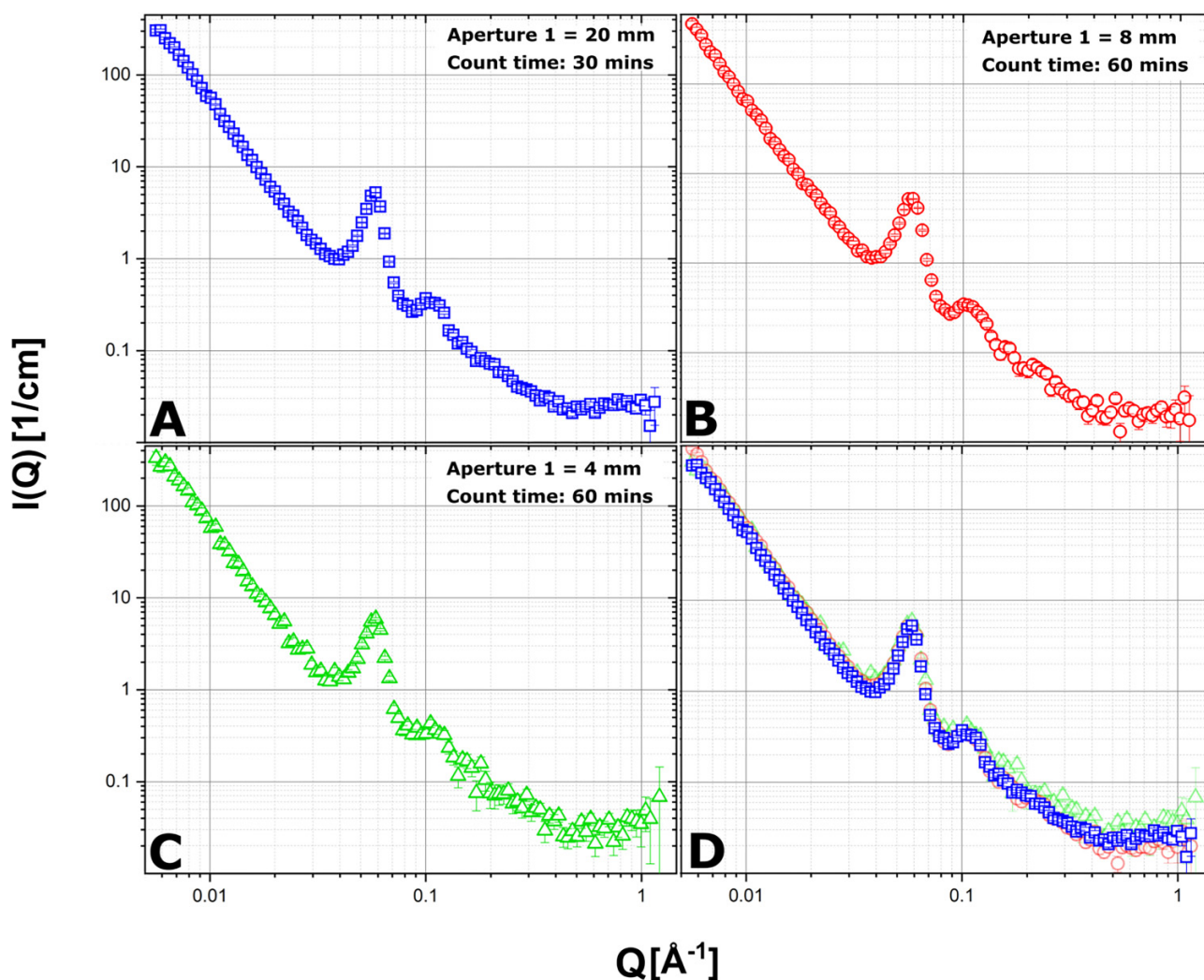
whereas the data for the reduced flux configurations were measured for 75  $\mu$ Hr ( $\sim$ 60 min). The results emphasize that even at these throttled fluxes one can still get analyzable data in a practical measurement time. Additional measurements were completed to stitch data for multiple hours, maxing out at about 6 h per sample. This is further reinforced by Table 2, where data with similar fractional error can be attained using Aperture 1 settings of 20 and 8 mm, by increasing the count time by a factor of 6. Therefore, by measuring the silicalite sample for 180 min, data were obtained with comparable fractional errors compared to 60 min of measurement at the LOQ configuration. Thus these measurements established the feasibility of using the 8 mm configuration (Fig. 2, red) to kickstart further comparisons of data quality as a function of flux and measurement time.

#### 3.2. Silver behenate

Another well-characterized sample measured was the long-chain fatty acid silver behenate [16]. This crystallizes with a lamellar structure, making it a useful standard for verifying the Q-scale and instrument resolution. Its distinct line shape and observable Bragg peaks in the low Q-range allows it to be used as another reference sample. It's disadvantage in SANS, compared to SAXS, is that it is a very weak scatterer. But this made for a worthwhile comparison with the silicalite above.

The silver behenate was measured in the two principal flux configurations and displayed the expected scattering curve with three reflections in the low-Q region but higher orders being lost in the incoherent background, as seen in Fig. 4. For the LOQ configuration the count time was 60 minutes, while the PC-CANS configuration count time was 360 min. In the LOQ configuration peaks were fit giving rise to Q-values of 0.1034 and 0.2029  $\text{\AA}^{-1}$ , compared to the PC-CANS configuration giving rise to similar peak locations of 0.1035 and 0.2099  $\text{\AA}^{-1}$ . Both sets of positions are consistent with those

**Fig. 3.** Comparison of the small angle neutron scattering (SANS) from silicalite MSU-H at different flux settings. The figure consists of four quadrants: (A) LOQ configuration with a 20 mm aperture, (B) prototype Canadian Compact Accelerator-driven Neutron Source (PC-CANS) configuration with an 8 mm aperture, (C) further restricted flux configuration with a 4 mm aperture, which results in approximately 25x less flux compared to the standard LOQ, and (D) overlay of all three configurations for direct comparison. Despite the reduction in flux, the potential viability of measuring this type of sample on a PC-CANS SANS is evident. Data was normalized to integrated proton charge.



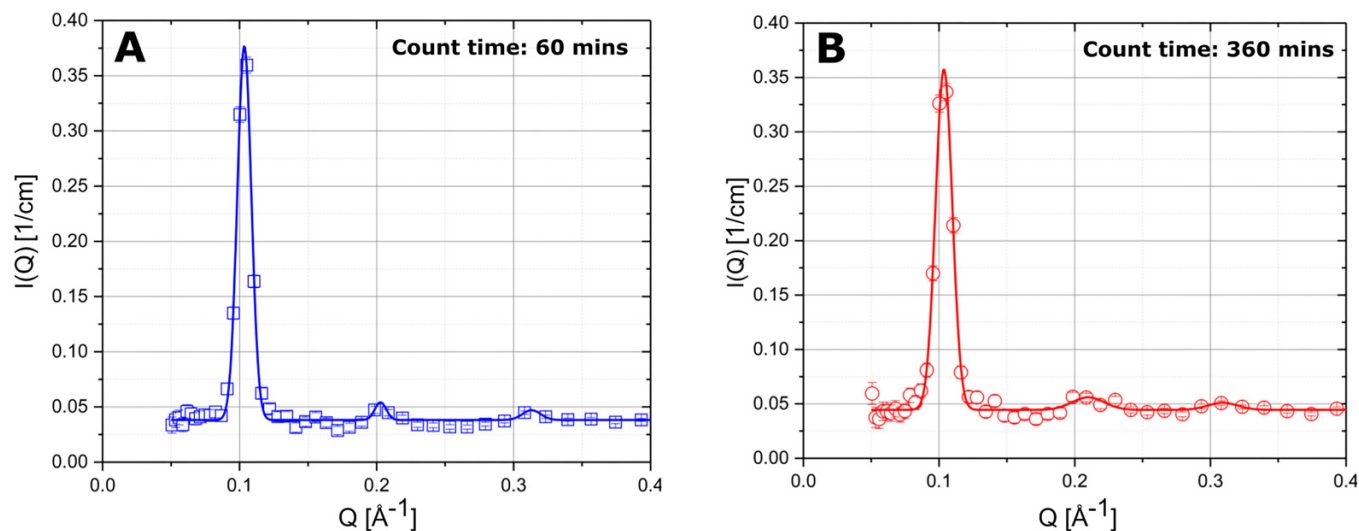
**Table 2.** Fractional error (FE) on the scattering intensity at various  $Q$ -values for silicalite samples at different aperture settings, where  $FE = \frac{\Delta I}{I}$ , and  $\Delta I$  is the uncertainty on the intensity measurement from the counting statistics.

Aperture 1 (mm)	Count time (mins)	Fractional error	Fractional error	Fractional error
		$Q (\text{Å}^{-1}) = 0.0087$	$Q (\text{Å}^{-1}) = 0.0825$	$Q (\text{Å}^{-1}) = 0.8173$
20	30	0.019	0.053	0.076
8	60	0.033	0.070	0.165
8	180	0.020	0.053	0.135
8	360	0.015	0.042	0.116
4	60	0.064	0.110	0.202

in the literature of 0.1086 and 0.2154  $\text{Å}^{-1}$ , although sample purity and storage conditions are known to affect the spacings [16]. Additionally, the associated error was in agreement with Table 2, where counting for six times longer allowed for comparable statistics. This shows by increasing the count

time by this modest factor it is possible to get comparable peak resolution on a potential PC-CANS SANS. It is important to note that for the purpose of this work these samples were used to look at general capability of the instrument and were not used for their calibration purposes, however it does

**Fig. 4.** Scattering curves for silver behenate measured using two different configurations. The left panel (A) shows the scattering curve obtained with the LOQ configuration, measured for 1 h, while the right panel (B) presents the curve from the prototype Canadian Compact Accelerator-driven Neutron Source configuration, measured for 6 h. The two curves are shown side-by-side for direct comparison, illustrating the differences in data quality and resolution between the two setups. The solid lines show Gaussian fits used to model the multiple silver behenate peaks. Data was normalized to integrated proton charge.



additionally show it will be possible to calibrate the PC-CANS SANS using established standards.

### 3.3. Phospholipid vesicles

One of the most important applications of SANS is in the area of life-sciences (biochemistry, biophysics, and biology). Herein we use example experiments from the area of lipid biochemistry. Structure and organization of liposomal systems are commonly investigated in the area of lipid biochemistry, specifically through the lens of a SANS instrument, due to the probe-free nature of the technique [17, 18]. The ability to investigate length scales ranging from 1 nm to more than 100 nm allows the extraction of a plethora of information, and specifically on the structure of the biomembrane [19]. Synthetic liposomes can therefore be used as a fundamental mimic for a variety of biomembrane systems, such as the cell membrane or other lipid-centric structures, such as pulmonary surfactant [20, 21]. These systems have gained world-wide visibility, specifically during the pandemic (Pfizer/BioNTech) and will be continuously of interest [22].

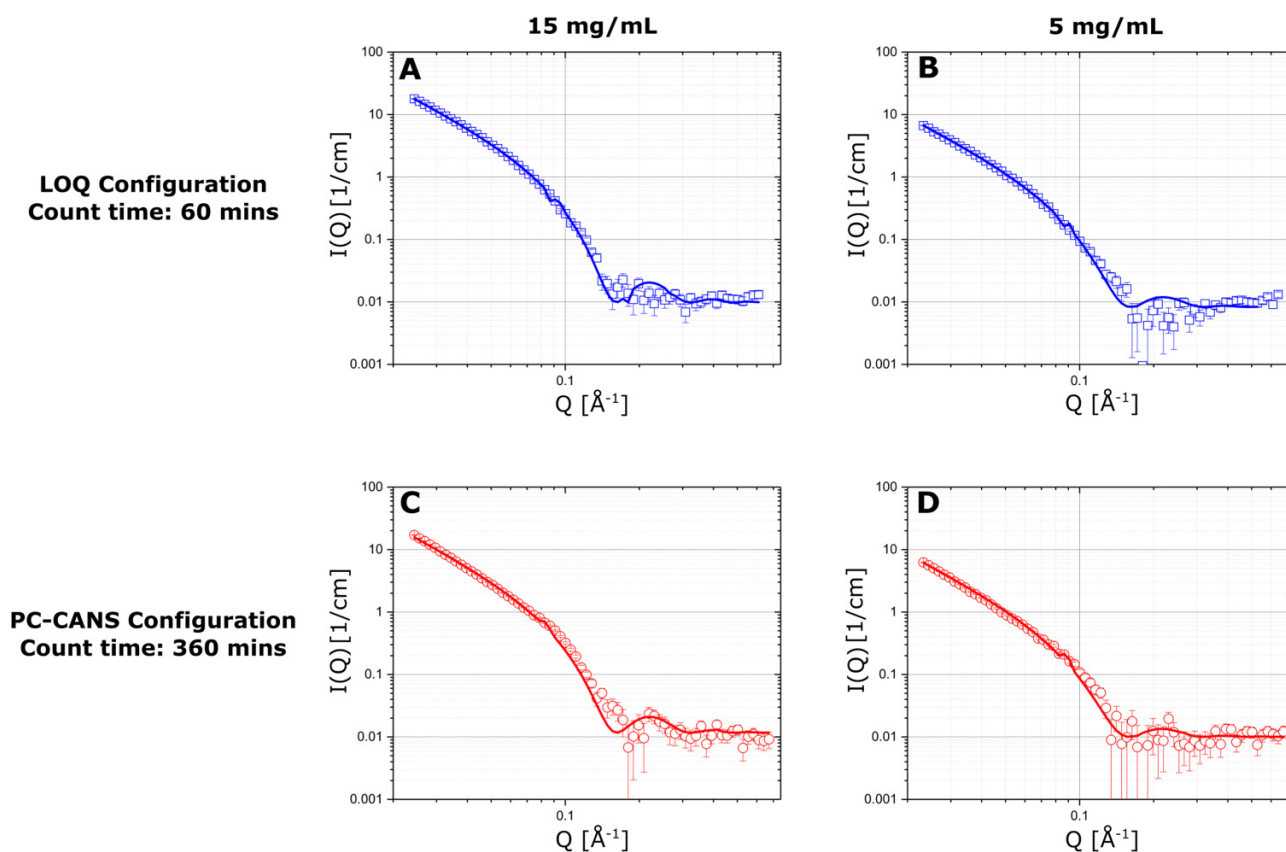
Thus, SANS provides a means to investigate the structure of biomembranes, with the ability to expand and examine how the addition of biologically relevant small molecules, such as peptides, influences their properties. As such, benchmarking such samples shows if a potential PC-CANS SANS instrument holds promise for advancing these important areas of research, and can act as a resource for investigators in the field.

In this part of the study, lipid vesicles composed of POPC were measured to extract the vesicle bilayer thickness, a key property of interest. Again, data were collected using the aforementioned LOQ and PC-CANS configurations. Figure 5 presents the scattering plots of the samples, which were measured at concentrations of 15 and 5 mg/mL to assess the sensi-

tivity of the measurements across the two configurations. As previously mentioned, sample count times were controlled based on the microamp-hour exposure. This roughly resulted in vesicle samples being measured in the LOQ configuration for one hour, whereas measurements in the PC-CANS mode were conducted over approximately six times that duration. For some researchers, this may reduce the appeal of exploring more uncertain or transient systems, especially if longer beamtime commitments pose a practical challenge. However, CANS-based instruments offer a clear advantage in this context: the relatively lower cost and more flexible access to beamtime make them especially attractive for longitudinal studies. Beyond temperature-dependent experiments, this includes investigations involving slow changes in structure (on the scale of hours or more), pressure, concentration, magnetic field, or other environmental parameters not requiring fine temporal resolution. In many cases, these kinds of studies—particularly on strongly scattering systems—would be more justifiable on a CANS instrument than at a spallation facility, where beamtime is more limited and expensive to operate. As such, CANS platforms alleviate some of the subscription overload associated with SANS at the world's brightest neutron sources and provide a compelling opportunity to expand the scope of neutron scattering research.

In the case of the POPC vesicles, bilayer thickness values are in agreement with each other after extraction of bilayer thickness values using SASView [23]. Vesicles initially measured in the LOQ configuration had a bilayer thickness of  $39.00 \pm 0.08$  and  $39.16 \pm 0.16$  Å, at 15 mg/mL and 5 mg/mL, respectively. The data obtained using the slower PC-CANS configuration yielded thicknesses of  $38.90 \pm 0.15$  and  $38.94 \pm 0.18$  Å, respectively, all within error. This is in agreement with literature of this well-studied POPC system [24, 25]. This further emphasizes the central theme that by increasing count

**Fig. 5.** Small angle neutron scattering data from POPC vesicles at 25 °C measured with the different flux settings. (A and B) In the LOQ configurations at 15 mg/mL and 5 mg/mL. (C and D) In the prototype Canadian Compact Accelerator-driven Neutron Source (PC-CANS) configuration. The solid lines are the optimized core-shell fits obtained using SASview. Error bars are indicative of one standard deviation. Data was normalized to integrated proton charge.



times, in this case by a factor of 6, one can obtain analyzable data, on a PC-CANS SANS, that will yield the same values, within error, of a workhorse instrument such as LOQ.

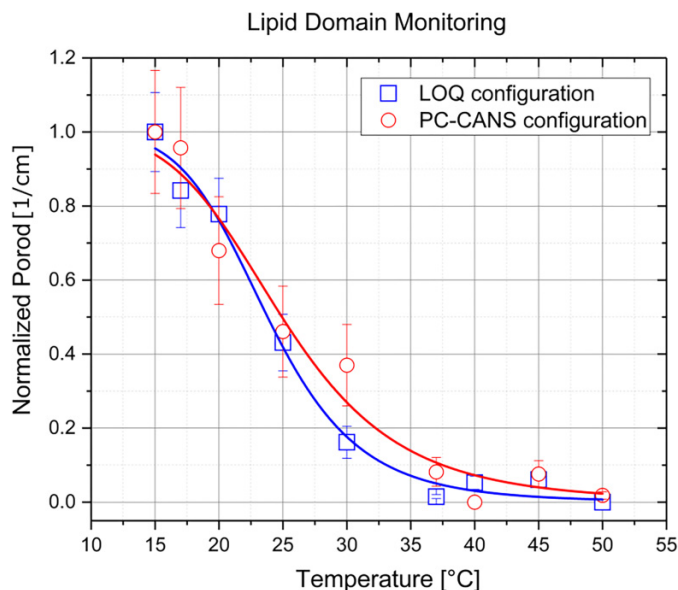
Other lipid-based experiments could also be investigated to show the versatility and value of a potential PC-CANS SANS for research purposes. In particular lipid domains are specialized, dynamic regions within biological membranes that segregate specific lipids and proteins, playing a crucial role in cellular processes such as signaling, protein sorting, and membrane fluidity, making their study through techniques like SANS invaluable for understanding membrane structure and function at the molecular level. Various studies exist looking at the formation of lipid domains in a variety of vesicle compositions, with domain formation largely being temperature dependent, and hence will typically entail a temperature series. This inclusion of a temperature series brings back into question the counting time required for a domains experiment. The same sample being measured over a course of many temperatures, for example 5 temperature points, will greatly increase the amount of time required on the beamline. This would lead from an experiment that would typically take approximately 5 h, to one requiring over a day of beamtime to complete. However, the beneficial part about benchmarking biological samples is that of the various dis-

ciplines that SANS can be used for, biological samples tend to be the least stable, when compared to other areas such as polymers or hard condensed matter.

Through contrast-matched SANS the presence and absence of domains can be monitored according to the protocol by DiPasquale et al. [26]. By measuring samples at various temperatures, ranging from 15 to 50 °C, one can measure and visualize the melting of domains as a loss scattering intensity. This process can be investigated for a variety of different lipid compositions to ultimately extract a melting temperature of these domains, or the addition of small molecules can be investigated to look at a stabilizing or destabilizing effect on lipid domains [26, 27]. These findings can further be used to attempt to modulate domain-related signaling pathways in aims of controlling physiological processes.

Using a previously-characterized domain composition of DPPC/POPC/Chol the presence of domains was monitored in both flux configurations. The scattering data is collected from various temperature points, and then analyzed in a model-independent manner. Through extracting the Porod invariant ( $Q^*$ ) at each temperature point, we were able to follow the total scattering intensity at each temperature and relate it back to the melting of domains, where higher scattering will be indicative of domain presence. Figure 6 depicts a

**Fig. 6.** Domain melting behaviour monitored through the normalized Porod invariants extracted from small angle neutron scattering data using the two configurations of interest. Fitting of the data using eq. (1) (continuous line) yields further information about the melting temperature of the domains of interest. The samples were technical replicates of the same stock sample, likely explaining the slight deviation in fit. Data was normalized to integrated proton charge. PC-CANS, prototype Canadian Compact Accelerator-driven Neutron Source.



plot of the normalized Porod invariant as a function of temperature, showing that as the temperature was raised the scattering arising from the system's contrast was deteriorating. By further modeling the contrast decay using a simple logistic function eq. (1) [26].

$$Q^* = \frac{Q^*_{\max}}{1 + \left(\frac{T}{T_m}\right)^r} \quad (1)$$

where  $Q^*_{\max}$  is the highest relative contrast achieved over the series, and  $T_m$  is the inflection of the curve, the point at which approximately one half of the lipid domains will be melted.  $r$  is the decay rate which encompasses a variety of more complex thermodynamic parameters that help dictate the melting process of the domains. Whilst these parameters were determined via a non-calorimetric process and should not be taken as absolutes, they still do provide useful insight about domain behaviour. As seen in Fig. 6, similar  $T_m$ ,  $23.8 \pm 0.4$  °C (LOQ) and  $24.9 \pm 0.8$  °C (PC-CANS), were extracted matching what is seen in literature for the same system [26].

These measurements indicate that the proposed PC-CANS SANS configuration on LOQ has significant potential in emulating data from a proven and trusted workhorse instrument like LOQ by increasing count time by a factor of 6. The configurations yield reproducible scattering curves for well-characterized samples in practical measurement durations,

but they also showed exceptional alignment with published data in lipid-based experimental analyses. This compelling evidence strengthens the case for the development and support of a potential PC-CANS system, showcasing its viability for real-world applications.

### 3.4. Peripheral improvements

The work here is based on conservative estimates of the proposed SANS instrument and PC-CANS performance. There are sources of improvements that we have not fully accounted for in our Conceptual Design Report [6]. Further improvements to the performance of our SANS instrument, when compared to LOQ, are difficult to predict computationally. For example, the effects of background on instrument performance has not been considered here, though the background on LOQ is known to be significantly worse than on the second-generation SANS instruments at ISIS. The LOQ detector is also 20 years old. Additionally, previous CANS-based SANS instruments have demonstrated a relatively lower sensitivity to background noise compared to those utilizing spallation or reactor sources [28, 29]. Newer technologies now exist, driven by the needs of the high-power spallation sources. Data collection is often not performed in an optimal fashion with the majority of users 'over-counting' their data.<sup>3</sup> Efforts made to increase the efficiency of data collection during a SANS experiment will increase user throughput independent of source optimizations. A key example of this is the use of artificial intelligence (AI) in experimental design, including determining when the optimal signal-to-noise is achieved in data collection [30, 31].

## 4. Concluding thoughts

The SANS instrument recommended for PC-CANS will be an invaluable tool for a wide range of scientific research that does not rely on the time resolution. We have demonstrated that measurements on the PC-CANS SANS will be of reasonable length, less than ten hours, for scientifically relevant model samples. From exploring colloids and lipid membranes to advancing stretchable semi-conducting polymers, ion-conducting polymers for fuel cells, food systems, long-wavelength magnetic structures, metal alloys, porous materials (eg, geological samples), and even certain superconducting flux lattices, its potential is truly exciting.

For Canadian researchers, this facility represents a game-changing opportunity. Currently, researchers face limited access to high-brightness, oversubscribed international facilities, even for experiments that do not require such brightness. By operating as a national user facility, this SANS instrument will not only meet Canada's growing demand for cold neutron SANS, but also empower researchers with hands-on experience. This will significantly enhance their ability to compete for, and fully leverage, precious beamtime at world-class neutron sources. This marks a major step forward for Canada's scientific community, fostering innova-

<sup>3</sup> Paul Butler at "Shaping the Future of Neutron Scattering in Canada: Workshop on Applications, Instruments, and Research Reactor Requirements".

tion, collaboration, and discovery. To answer the questions posed in the title, “Would a SANS on PC-CANS be worth it?” the answer is undoubtedly yes.

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### Data availability

Data are available at here: <https://doi.org/10.5286/ISIS.E.RB2400003>.

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Data curation: MD, DDM

Formal analysis: MD, DDM

Funding acquisition: DM

Investigation: MD, SC, SK, DM

Methodology: SK

Resources: SK, DM

Supervision: SK

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## Competing interests

The authors declare there are no competing interests.

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