Supporting Information

Comparability of Raman Spectroscopic Configurations:
A Large Scale Cross-Laboratory Study

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Design of the Ring Trial

We describe here the first round of a ring trial which was designed to assess the cross-setup comparability in Raman spectroscopy among a wide variety of laboratories in Europe. The samples consisted of well-known standards in Raman spectroscopy: a NeAr glow lamp, a paracetamol powder (also known as acetaminophen), a polystyrene petri dish, cyclohexane, and two biological example substances, agar and gelatine.

This selection was based on the following guiding principles:

- The NeAr glow lamp emits at well-known wavelengths [1, 2]. This allows to check the wavelength/wavenumber calibration of the spectrograph independently of the calibration of the excitation laser wavelength. In addition, the emission lines are very narrow: their line width is negligible compared to the spectral resolution of all participating instrument configurations (see Table S2). This allows to directly measure the instrument line shape and the spectral resolution of the spectrograph [3]. NeAr glow lamps are both readily available and give a large number of lines across the wavelength ranges covered by Raman spectrometers with excitation between 514 and 785 nm.

- Paracetamol, polystyrene and, if available, cyclohexane are widely-used standard substances for calibrating the spectral axis (wavenumber axis) of Raman spectrometers. They are also substances for verifying the wavenumber calibration
according to the European Pharmacopoeia [4] and ASTM E1840 [5]. Having more than one such substances allows to set up a wavenumber calibration based on one substance and assess the quality of the obtained calibration with the remaining substances. Paracetamol is polymorphic [6], and the Pharmacopoeia specifies that monoclinic paracetamol has to be measured [4]. Participants were shown Raman spectra of the monoclinic and orthorhombic modifications in the workshop that finalized the sample decisions and were reminded to not melt the sample as that may result in orthorhombic paracetamol.

- For cyclohexane the intensity ratios of the integral intensities of several bands are available in the literature [1, 2]. It can be considered to be intensity standard and used to assess how comparable spectra are in terms of the Raman intensities.
- Care was taken to select substances that do not show resonance enhancement with any of the excitation wavelengths in the participants’ Raman configurations.
- The ring trial samples should serve to assess the performance characteristics needed for both quantitative (regression) and qualitative (classification) biospectroscopic tasks.
- The optical configurations of the labs participating in Raman4clinics varied from highly confocal and high spatial resolution to the fiber-optic setups with lower spatial resolution. In this way, we expected to take into account the influence of instrumental configurations on the spectral reproducibility. We ensured that the samples were homogenous at these scales to allow instrument comparison across a wide range of spatial resolutions. To check any intensity variations in a dataset, an isotropic liquid like cyclohexane is the best choice, followed by the polystyrene petri dish (which is a clear substrate of sufficient size but it may exhibit local alterations due to the production process). The paracetamol powder with a crystal size that allows to measure a particular crystal face with high spatial resolution Raman configurations might be used as well. In addition, we chose agar and gelatine gels as example substances for biological materials. Both can be prepared as gels to be measured across the whole range of spatial resolutions. These two substances allow to benchmark the signal intensity and the signal-to-noise ratio for biological samples like bacteria, cells or tissues. With green excitation (514 and 532 nm), however, they exhibit a strong background and a Raman measurement will be successful only if it is performed fully confocal.
- In terms of the polarization, the participants’ instrument configurations also ranged from microscopic to fiber optical setups, which differed in their polarization dependency. The polarization effect is out of scope of our analysis.

Materials

NeAr glow lamps were purchased and already equipped with an appropriate resistor for 230V. As both electric safety regulations and plug standards vary across the participants’ countries, participants were asked to have a local electrician connection to the NeAr glow lamp according to the customs.

All portions of paracetamol were taken from the same batch of pharmaceutical grade paracetamol (Mallinckrodt Inc, USA/Caelo lot 15075707).
One batch of polystyrene petri dishes was used both as samples and containers for the other substances.

Agar (Kobe I Art.-Nr. 5210.2, Carl Roth, Germany, as 10 w% solution) and gelatine (bovine skin, type B, Sigma Germany, G9391-100G, lot SLBM7200V, as 20 % solution) were dissolved in distilled water under stirring for at least 1 h. To avoid contamination by growing microorganisms over time, the solution was sterilized in the autoclave. The sterilized solution was kept at 60°C to be handled further as homogenous liquid. It was pipetted into 2mL Eppendorf tubes under sterile conditions and allowed to cool down. Retained samples were stored at room temperature as sterilization check. A check after 4 weeks revealed no growing microorganisms, thus, samples were shipped sterile.

In addition, the participating labs were encouraged to measure and submit spectra of their own cyclohexane: due to transport restrictions on hazardous materials we decided to not ship cyclohexane.

Measurement Instructions to Participants

Since the participants’ instrument configurations varied widely, it did not make sense to prescribe excitation power and [total] exposure time. Participants were therefore instructed to select excitation power, exposure time, coadditions/average of spectra and objective and to report these parameters. We requested to upload at least 10 spectra with the integral intensity over a specific band having signal-to-noise ratio SNR (calculated as mean integral intensity divided by the standard deviation of integral intensity over the submitted spectra after local baseline correction, as defined by Eq. (S3.3)) better than a threshold which was pre-defined for each substance and each band, depending on red (630 – 785 nm) vs. green (514 – 532 nm) excitation, see table S1. The bands were selected to both have high intensity and be sufficiently separated from any other bands so that local baseline correction and band integral intensity could be calculated also for configurations with low spectral resolution.

Table S1: Acceptable signal-to-noise ratio for specific band integral intensities across the at least 10 submitted spectra

<table>
<thead>
<tr>
<th>Sample</th>
<th>band(s)</th>
<th>SNR 532 nm laser</th>
<th>SNR 785 nm laser</th>
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<td>NeAr glow lamp</td>
<td>626.56 nm</td>
<td>500</td>
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<tr>
<td></td>
<td>878.2 nm</td>
<td></td>
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<tr>
<td>cyclohexane</td>
<td>801 cm⁻¹</td>
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<tr>
<td>paracetamol</td>
<td>1169 cm⁻¹</td>
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<td>250</td>
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<td>polystyrene (petri dish)</td>
<td>1451 cm⁻¹</td>
<td>500</td>
<td>250</td>
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<td>gelatine</td>
<td>1220 – 1490 cm⁻¹</td>
<td>50</td>
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<tr>
<td>agar</td>
<td>970 cm⁻¹</td>
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These high SNRs were chosen on the one hand to allow data analyses which need high-quality spectra (e.g., measuring band positions and band widths). During the ring trial, some participants had difficulties in achieving this SNR with normal coadditions/averaging due to short-term fluctuations/intensity drift. We therefore relaxed the requirements and allowed participants to upload series of more spectra as long as coadding random spectra of the series lead to an SNR passing the limit across at least 10 such coadded spectra.
Spectral Pre-processing

Here we describe the details of the spectral pre-processing steps. To start, the spike removal was achieved via a comparison between every two Raman spectra from the same substance. Any spikes were detected where the Raman intensity of one spectrum is abnormally higher than it is for the other spectrum. The detected spike regions were replaced with the intensities of the other Raman spectrum after correcting the baseline offset. In the next step, a wavenumber calibration function was derived based on the spectra of paracetamol for each setup. To do so, the position of each known Raman band of paracetamol (see Figure S4 (b)) was estimated as the mean position of a Gaussian curve fitted from the neighborhood of this band. Thereafter, a third order polynomial was fitted between these measured band positions \( \tilde{\nu}_i \) and their correct values \( \tilde{\nu}_i^0 \) (Eq. (S1)). This calibration function was then interpolated onto the whole spectral region and used to calibrate the wavenumber axis for all substances: agar, gelatine, paracetamol, cyclohexane, and polystyrene. Thereafter, all spectra were interpolated to an equidistant wavenumber grid of 1 cm\(^{-1}\) and baseline corrected via the sensitive nonlinear iterative peak (SNIP) clipping algorithm [7]. In the end, we normalized the Raman intensities against the \( I_2 \) norm of the spectral region \( R: 730 \leq \nu \leq 1700 \) cm\(^{-1}\) (see Eq. (S2)).

\[
\nu_i^0(\tilde{\nu}_i) = a_0 + a_1 \cdot \tilde{\nu}_i + a_2 \cdot \tilde{\nu}_i^2 + a_3 \cdot \tilde{\nu}_i^3 \quad \text{Eq. (S1)}
\]

\[
I^n(\tilde{\nu}_i) = \frac{I(\tilde{\nu}_i)}{\sqrt{\sum_{j \in R} I(\tilde{\nu}_j)^2}} \quad \text{Eq. (S2)}
\]

**Signal Noise Ratio**

In the following, we formulated the three different calculations of the signal noise ratio in this project. Here we denoted a Raman spectrum and the estimated noise as \( I \) and \( I_n \), respectively. The terms \( I_i^p \) and \( A_i^p \) represent the integrated and maximal intensity of a specific Raman band \( p \) in the \( i^{th} \) spectrum, respectively. In particular, the SNR\(_1\) and SNR\(_2\) were used for the results shown in Figure 1 and S8, respectively, while SNR\(_3\) was calculated for presorting before being uploaded.

\[
\text{SNR}_1 = \frac{\text{mean}(I)}{\text{sd}(I_n)} \quad \text{Eq. (S3.3)}
\]

\[
\text{SNR}_2 = \frac{\text{mean}(I_i^p)}{\text{sd}(I_i^p)}, i = 1, 2, \ldots, 10 \quad \text{Eq. (S3.2)}
\]

\[
\text{SNR}_3 = \frac{\text{mean}(A_i^p)}{\text{sd}(A_i^p)}, i = 1, 2, \ldots, 10 \quad \text{Eq. (S3.1)}
\]
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Figure S1: Error in the measurement of the setup ID25. (left) Difference of each two subsequent wavenumbers, the pattern within the region of 1500-2600 cm⁻¹ shows irregular oscillation in the recorded wavenumber positions. (right) The irregular oscillation resulted in errors in the measured Raman intensities.
Figure S2: Mean spectra and standard deviation spectra of agar measured with different laboratory setups. For clarity the spectra are offset in the y-axis.
Figure S3: Mean spectra and standard deviation spectra of gelatine measured using different laboratory setups. For clarity the spectra are offset in the y-axis.
Figure S4: (a) Mean spectra and standard deviation spectra of paracetamol. For clarity the spectra are offset in the y-axis. (b) Enlarged representative spectra where the peaks used for the calculation of peak shifts are highlighted in green.
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Figure S7: Mean spectra and standard deviation spectra of the NeAr lamp. (a) Measurements on setup with 514/515/532 nm laser source. (b) Measurement with 785 nm laser source. The spectra were normalized against their respective maximum.
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Figure S9: Results of SNR for (a) agar and (b) gelatine. The colour shades represent the setups with different excitation wavelengths. The SNR is calculated from 10 spectra based on one single Raman band. The band used for this calculation is marked in the caption of both plots. Please note that the SNR here is calculated according to Eq. (S3.2), which is different to the SNR used for data pre-sorting (Eq. (S3.3)).
Figure S10: Results of peak shifts for cyclohexane without (a) and with (b) wavenumber calibration. The colour shades represent the setups with different excitation wavelengths. The wavenumber calibration was performed if there was paracetamol measured on the same setup. Therefore, less measurements are shown for the calibrated results than without wavenumber calibration.
Figure S11: (a) Results of FWHM calculated from cyclohexane based on the peak at 1028 cm\(^{-1}\). (b) Results of FWHM calculated from NeAr based on the emission lines at 626.56 and 878.2 nm for the laser sources at 514/532 and 785 nm, respectively. The colour shades represent the setups with different source wavelengths.
Figure S12: Mean absolute deviation with respect to the nominal spectral resolution of different setups. Rows (a-c) show results from paracetamol, polystyrene, and cyclohexane, respectively. The left and right columns give results without and with wavenumber calibration, respectively.
Figure S13: FWHM with respective to the nominal spectral resolution. The Raman band selected for the FWHM calculation was marked in the plots for each substance.
Figure S14: Results of the peak ratio between the cyclohexane peaks at 1444 and 801 cm\(^{-1}\). The curved arrows in brown show the paired results, pointing to the results with intensity calibration.
References