Data Article

Dataset of serum proteomic spectra from tuberculosis patients detected by Raman spectroscopy and surface-enhanced Raman spectroscopy

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Abstract

In this data article, we present Raman spectroscopy (RS) and surface-enhanced Raman spectroscopy (SERS) data obtained using an InVia Reflex confocal Raman microscope (Renishaw; Wotton-under-Edge, UK) and processed using WiRE™ 4.2 software. The data include RS and SERS spectra detected, after removal of albumin, from the serum proteome of tuberculosis (TB) patient categories and controls (active tuberculosis; ATB, latent tuberculosis; LTBI, TB-exposed persons with undetected infection; EC, healthy controls; HC) using 532 nm and 785 nm laser wavelengths for RS and SERS, respectively. The RS and SERS data had high reproducibility (SERS: $R^2 = 0.988$, RS at 785 nm: $R^2 = 0.972$, RS at 532 nm: $R^2 = 0.9150$). This data can be used for analysis of proteomic spectra based on RS and SERS for TB diagnosis and can also be compared to other populations. The spectral dataset based on
normal, healthy control groups might be used as the control data for analysis of other diseases using RS and SERS approaches.

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Specifications Table

| Subject                        | Spectroscopy, Infectious Diseases, Proteomics |
|--------------------------------|----------------------------------------------|
| Specific subject area          | Raman Spectroscopy (RS) and surface-enhanced Raman spectroscopy (SERS) in serum protein samples detected among tuberculosis categories |
| Type of data                   | Raw and analysed data                         |
| How data were acquired         | InVia Reflex confocal Raman microscope (Renishaw; Wotton-under-Edge, UK) and WiRE™ 4.2 software (Renishaw, UK) were used for data acquiring. In-house developed SERS chips (NECTEC, Thailand) were used for SERS analysis. |
| Data format                    | [.xlsx] and [.tiff]                           |
| Parameters for data collection | RS detected at 532 and 785 nm laser wavelengths and SERS detected at 785 nm laser wavelength. |
| Description of data collection | Protein fingerprint spectra based on RS and SERS were collected from serum proteome of 118 samples including 26 samples of active tuberculosis, 26 samples of latent tuberculosis infection, 34 samples of early clearance and 38 samples of healthy controls. |
| Data source location           | Department of Microbiology, Faculty of Medicine, Khon Kaen University, Khon Kaen, Thailand |
| Data accessibility             | Data is available with this publication      |

Value of the Data

- This dataset provide serum proteomic spectra from individuals with latent tuberculosis (TB) and those with active TB based on Raman Spectroscopy (RS) and SERS. This is the only serum proteomic spectral dataset of latent TB in a public database.
- These data may be relevant for other researchers who (i) analyze the serum proteome based on RS and SERS, (ii) have a focus on TB diagnosis, especially for distinguishing between active and latent TB.
- The dataset might be used for TB diagnostic applications by distinguishing among TB disease categories including active TB, latent TB, TB-exposed persons with undetected infection and healthy controls based on RS and SERS spectra.
- The spectral dataset of the normal healthy control groups might be used as the control data for studies on other diseases based on Raman spectroscopy analysis.

1. Data

In this report, we present data of serum proteomic spectra detected among TB-infection categories using both Raman spectroscopy (RS) and surface-enhanced Raman spectroscopy (SERS). The TB-infection categories included unexposed individuals without infection (healthy controls; HC), exposed individuals without infection (early clearance; EC), those with latent infection (LTBI) and those with active TB disease (ATB). The protocol to acquire the dataset was approved by the Khon Kaen University Ethics Committee in Human Research (Ethics number HE611116).

The presented data include raw data of protein fingerprints detected among TB catagories (Supplementary Table S1). The high reproducibility of the data detected from both RS and SERS is shown in Fig. 1 and Table 1. The reproducibility of protein samples measured using SERS ($R^2 = 0.988$) was slightly higher than that of RS at 532 nm ($R^2 = 0.915$) and at 785 nm ($R^2 = 0.972$) (Fig. 1 and Table 1).
Fig. 1. Reproducibility of Raman spectroscopy at 532 nm and 785 nm and SERS. A high correlation was found among sample replicates (average of 120 comparisons from 16 replicates) in Raman spectroscopy at 532 nm and 785 nm and SERS. The values at the upper left of each panel show average of R² from each pair (all data are shown in Table 1).

Table 1

| Replications | RS | SERS | Comparisons | RS | SERS | Comparisons | RS | SERS |
|--------------|----|------|-------------|----|------|-------------|----|------|
| Rep1 vs Rep2 | 0.94 | 0.9 | Rep5 vs Rep10 | 0.98 | 0.99 | Rep3 vs Rep14 | 0.98 | 0.99 |
| Rep1 vs Rep3 | 0.94 | 0.92 | Rep6 vs Rep10 | 0.97 | 1 | Rep4 vs Rep14 | 0.97 | 0.99 |
| Rep2 vs Rep3 | 0.95 | 0.99 | Rep7 vs Rep10 | 0.92 | 1 | Rep5 vs Rep14 | 0.98 | 0.99 |
| Rep1 vs Rep4 | 0.96 | 0.9 | Rep8 vs Rep10 | 0.98 | 0.97 | Rep6 vs Rep14 | 0.98 | 1 |
| Rep2 vs Rep4 | 0.95 | 0.99 | Rep9 vs Rep10 | 0.98 | 1 | Rep7 vs Rep14 | 0.94 | 1 |
| Rep3 vs Rep4 | 0.96 | 0.99 | Rep11 vs Rep11 | 0.94 | 0.9 | Rep8 vs Rep14 | 0.98 | 0.97 |
| Rep1 vs Rep5 | 0.96 | 0.89 | Rep2 vs Rep11 | 0.96 | 0.99 | Rep9 vs Rep14 | 0.98 | 1 |
| Rep2 vs Rep5 | 0.96 | 0.99 | Rep3 vs Rep11 | 0.98 | 0.99 | Rep10 vs Rep14 | 0.98 | 1 |
| Rep3 vs Rep5 | 0.97 | 0.99 | Rep4 vs Rep11 | 0.97 | 0.99 | Rep11 vs Rep14 | 0.98 | 0.99 |
| Rep4 vs Rep5 | 0.97 | 0.99 | Rep5 vs Rep11 | 0.98 | 0.99 | Rep12 vs Rep14 | 0.98 | 0.99 |
| Rep1 vs Rep6 | 0.96 | 0.89 | Rep6 vs Rep11 | 0.98 | 0.99 | Rep13 vs Rep14 | 0.92 | 0.99 |
| Rep2 vs Rep6 | 0.96 | 0.99 | Rep7 vs Rep11 | 0.93 | 0.99 | Rep1 vs Rep15 | 0.64 | 0.91 |
| Rep3 vs Rep6 | 0.96 | 0.99 | Rep8 vs Rep11 | 0.98 | 0.98 | Rep2 vs Rep15 | 0.74 | 0.99 |
| Rep4 vs Rep6 | 0.97 | 0.99 | Rep9 vs Rep11 | 0.98 | 0.99 | Rep3 vs Rep15 | 0.76 | 0.99 |
| Rep5 vs Rep6 | 0.98 | 0.99 | Rep10 vs Rep11 | 0.99 | 0.99 | Rep4 vs Rep15 | 0.7 | 0.99 |
| Rep1 vs Rep7 | 0.94 | 0.87 | Rep1 vs Rep12 | 0.95 | 0.92 | Rep5 vs Rep15 | 0.71 | 0.99 |
| Rep2 vs Rep7 | 0.94 | 0.99 | Rep2 vs Rep12 | 0.96 | 0.99 | Rep6 vs Rep15 | 0.7 | 0.99 |
| Rep3 vs Rep7 | 0.92 | 0.99 | Rep3 vs Rep12 | 0.97 | 0.99 | Rep7 vs Rep15 | 0.67 | 0.99 |
| Rep4 vs Rep7 | 0.93 | 0.99 | Rep4 vs Rep12 | 0.97 | 0.99 | Rep8 vs Rep15 | 0.73 | 0.97 |
| Rep5 vs Rep7 | 0.94 | 0.99 | Rep5 vs Rep12 | 0.97 | 0.99 | Rep9 vs Rep15 | 0.76 | 0.99 |
| Rep6 vs Rep7 | 0.94 | 0.98 | Rep6 vs Rep12 | 0.97 | 0.99 | Rep10 vs Rep15 | 0.77 | 0.99 |
| Rep1 vs Rep8 | 0.95 | 0.84 | Rep7 vs Rep12 | 0.94 | 0.99 | Rep11 vs Rep15 | 0.75 | 0.99 |
| Rep2 vs Rep8 | 0.96 | 0.97 | Rep8 vs Rep12 | 0.97 | 0.97 | Rep12 vs Rep15 | 0.74 | 0.99 |
| Rep3 vs Rep8 | 0.97 | 0.97 | Rep9 vs Rep12 | 0.97 | 0.99 | Rep13 vs Rep15 | 0.68 | 0.98 |
| Rep4 vs Rep8 | 0.97 | 0.97 | Rep10 vs Rep12 | 0.97 | 0.99 | Rep14 vs Rep15 | 0.74 | 0.99 |
| Rep5 vs Rep8 | 0.98 | 0.98 | Rep11 vs Rep12 | 0.98 | 0.99 | Rep1 vs Rep16 | 0.94 | 0.96 |
| Rep6 vs Rep8 | 0.98 | 0.98 | Rep12 vs Rep13 | 0.82 | 0.85 | Rep2 vs Rep16 | 0.95 | 0.96 |
| Rep7 vs Rep8 | 0.93 | 0.98 | Rep2 vs Rep13 | 0.84 | 0.99 | Rep3 vs Rep16 | 0.97 | 0.97 |
| Rep9 vs Rep9 | 0.94 | 0.87 | Rep3 vs Rep13 | 0.81 | 0.98 | Rep4 vs Rep16 | 0.96 | 0.96 |
| Rep2 vs Rep9 | 0.96 | 0.99 | Rep4 vs Rep13 | 0.82 | 0.99 | Rep5 vs Rep16 | 0.97 | 0.95 |
| Rep3 vs Rep9 | 0.97 | 0.99 | Rep5 vs Rep13 | 0.81 | 0.99 | Rep6 vs Rep16 | 0.97 | 0.95 |
| Rep4 vs Rep9 | 0.96 | 0.99 | Rep6 vs Rep13 | 0.82 | 0.99 | Rep7 vs Rep16 | 0.93 | 0.94 |
| Rep5 vs Rep9 | 0.98 | 0.99 | Rep7 vs Rep13 | 0.87 | 0.99 | Rep8 vs Rep16 | 0.97 | 0.91 |
| Rep6 vs Rep9 | 0.97 | 1 | Rep8 vs Rep13 | 0.81 | 0.98 | Rep9 vs Rep16 | 0.96 | 0.94 |
| Rep7 vs Rep9 | 0.93 | 1 | Rep9 vs Rep13 | 0.81 | 0.99 | Rep10 vs Rep16 | 0.97 | 0.95 |
| Rep8 vs Rep9 | 0.97 | 0.98 | Rep10 vs Rep13 | 0.8 | 0.99 | Rep11 vs Rep16 | 0.97 | 0.95 |
| Rep1 vs Rep10 | 0.93 | 0.89 | Rep11 vs Rep13 | 0.8 | 0.99 | Rep12 vs Rep16 | 0.97 | 0.97 |
| Rep2 vs Rep10 | 0.95 | 0.99 | Rep12 vs Rep13 | 0.83 | 0.98 | Rep13 vs Rep16 | 0.81 | 0.92 |
| Rep3 vs Rep10 | 0.98 | 0.99 | Rep1 vs Rep14 | 0.95 | 0.88 | Rep14 vs Rep16 | 0.97 | 0.94 |
| Rep4 vs Rep10 | 0.96 | 1 | Rep2 vs Rep14 | 0.96 | 0.99 | Rep15 vs Rep16 | 0.71 | 0.96 |
2. Experimental design, materials, and methods

2.1. Field collection of samples

In total, 118 serum samples including 26 samples of ATB, 26 samples of LTBI, 34 samples of EC and 38 samples of HC from the biobank of the Department of Microbiology, Faculty of Medicine, Khon Kaen University [1] were used. A diagnosis of ATB was based on clinical symptoms and positive evidence from a molecular test (Xpert MTB/RIF, Cepheid, Sunnyvale, CA, USA), acid-fast bacillus staining or bacterial culture. LTBI cases were defined based on a positive result of the QuantiFERON-TB Gold test (QFT) from healthy TB-exposed (persons having close contact with an ATB patient, such as working in TB wards for at least 6 months). The EC category was defined based on a negative result of the QFT in individuals having contact with ATB patients. Healthy controls (HC) were defined as apparently healthy persons with no evidence of TB exposure and having a negative result of the QFT.

2.2. Sample preparation

Albumin was excluded from each serum sample using protein filtration columns and centrifugation. Protein concentrations were measured using the Bradford protein assay and 0.8 mg of each protein sample were dropped onto aluminum foil. The samples were left to air dry for 3 minutes and detected using RS and SERS.

2.3. Protein fingerprint spectra collection and analysis

Raman Spectroscopy readings were taken on an InVia Reflex confocal Raman microscope (Renishaw; Wotton-under-Edge, UK) in a range of 179–1926 cm\(^{-1}\) for a 532 nm laser and 508–1632 cm\(^{-1}\) for a 785 nm laser. Data were generated based on RS detected at 532 and 785 nm laser wavelengths and SERS detected at 785 nm laser wavelength with 16 area points of detection in each sample. WiRE\textsuperscript{TM} 4.2 software was used for data processing. To test the reproducibility of RS and SERS data, the average R\(^2\) score of 120 comparisons among 16 replications (detected from 1 to 16 area points) were calculated from 1010 peak positions in a sample from a randomly selected ATB case using the corrgram package in the R programming language. All SERS chips were developed by our group (NECTEC, Thailand). However, due to a shortage of SERS chips, we pooled the serum protein samples to match the available number of SERS chips.

Funding

This work was supported by Invitation Research 2018, Faculty of Medicine (IN61210); and Research Fund for Supporting Lecturer to Admit High Potential Student to Study and Research on His Expert Program Year 2015 (581H223), Graduate Studies, Khon Kaen University.

Ethics approval and consent to participate

The specimens from the biobank of the Department of Microbiology, Faculty of Medicine, Khon Kaen University. The protocol to obtain the dataset was approved by the Khon Kaen University Ethics Committee in Human Research (Ethic number HE611116).

Acknowledgments

We thank the National Center for Genetic Engineering and Biotechnology (BIOTEC) and the National Science and Technology Development Agency (NSTDA) for laboratory support during the Raman spectroscopy and SERS analysis. We would like to acknowledge Prof. David Blair for editing the MS via Publication Clinic KKU, Thailand.
Conflict of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.dib.2019.104891.

Reference

[1] D. Nonghanphithak, W. Reechaipichitkul, W. Namwat, V. Lulitanond, V. Naranbhai, K. Faksri, Genetic polymorphisms of CCL2 associated with susceptibility to latent tuberculous infection in Thailand, Int. J. Tuberc. Lung Dis. 20 (2016) 1242–1248, https://doi.org/10.5588/ijtld.16.0017.