MicrobioRaman: An open-access web repository for microbiological Raman spectroscopy data

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Our edits and additions are highlighted in red. Please see also the clean version (Lee et al._correspondence_ms_clean.docx).

To the editor: Raman spectroscopy (a type of vibrational spectroscopy) relies upon inelastic scattering, in which, after interaction with molecules in a sample, the wavelength of the scattered light differs from the wavelength of the incident light, which is typically provided by a laser. This shift in wavelength differs according to the type of molecules and their vibrational modes, allowing for the analysis of complex sample chemistry in a non-destructive manner (**Fig. 1a**). When Raman spectroscopy is applied for the measurement of microbiological samples, specific Raman peaks at different wavenumbers indicate the presence of macromolecules such as carbohydrates, proteins, lipids, nucleic acids, and pigments(some refs to be added). Recent advances in technology and data analysis now enable the investigation of molecular composition at the resolution of a single microorganism with high measurement sensitivity (**Fig. 1a**). By measuring the presence of peaks corresponding to specific macromolecules or differences in spectral shape, peak position, and relative intensity of peaks, and often in conjunction with complementary techniques, such as stable isotope probing (SIP)[1], fluorescence *in situ* hybridization (FISH)[2], or -omics(ref), Raman spectroscopy enables investigation of cell identity and phenotypes. This analytical approach is increasingly being employed to address important questions in both fundamental and applied microbiology (**Fig. 1b**). Notable applications include the measurement of microbial diversity in terms of cell identity, metabolic phenotype, and functional role within complex microbial communities. Raman spectroscopy is also allowing researchers to untangle the complexity of microbial communities, by allowing for the tracking of molecular interactions, such as mutualistic, competitive, or antagonistic exchange between microorganisms or between a microorganism and its host, and the interactions between microorganisms and their environment. In comparison to other technologies offering similar capabilities (enabling analysis of molecular composition and structure of samples, for instance, FTIR[3], cryogenic electron microscopy (cryo–EM)[4,5], nanoscale secondary ion mass spectroscopy (nanoSIMS)[6], nuclear magnetic resonance (NMR) spectroscopy[7]), the versatility in sample size and analysis conditions (in liquid phase or dry form) and the ability to measure live microorganisms render Raman spectroscopy applicable to diverse sample types, ranging from large nematodes (and beyond) to minuscule viruses measuring a few tens of nanometres, collected from various environments spanning oceans, soils, mammalian guts, and even other planets like Mars (see refs. [1,8–11] for comprehensive reviews about Raman technologies and applications in microbiology). To provide a foundation for this growing field, here we announce the establishment of a novel open-access repository for sharing of microbiological Raman data within the community and present a set of reporting standards.

Despite the potential of Raman spectroscopy in microbiology, the reporting of analytical methods and data for microbiological systems has evolved in a haphazard manner and progress in the field is hindered by the lack of both a set of standards for data reporting and a common database to deposit microbiological Raman data. Raman data from microorganisms is relatively complex to analyse because proper interpretation is dependent upon (i) biological context, (ii) experimental conditions, and (iii) data processing. We briefly discuss these three aspects here — see refs. [1,8–11] for detailed information.

Individual Raman spectra from microbiological samples, consisting of discretized wavenumbers (typically measured in cm^{-1}) and corresponding Raman scattering signals, typically encompass many (often overlapping) peaks that represent chemical bonds of diverse types of macromolecules. Identification of the source of each peak often depends on the biological context; for example, a peak at 1,570 cm^{-1} typically corresponds to C–C stretching of nucleic acids when analysing microorganisms more generally, but to calcium dipicolinic acids (CaDPA) when measuring endospore-forming bacteria[8]. Moreover, SIP or FISH, often coupled to Raman measurements to track metabolic exchange or identify microorganisms of interest, induce a red shift of Raman peaks (i.e., peak positions move to lower wavenumbers) or a change in overall spectral shape, respectively, adding further complexity to the interpretation of microbiological Raman data.

Experimental conditions further complicate the analysis of microbiological Raman data. Compared to Raman measurements in research fields in which samples are in the solid state (often the case in material science or electrical engineering) or target cells are relatively large (a few tens of micrometres, as in biomedical engineering), samples in microbiology often contain a diversity of molecules at relatively low concentrations (diverse cell components, with the majority in liquid phase) and target cells are rather small (e.g., bacteria or archaea ranging down to a few hundreds of nanometres). Microbiological measurements are thus substantially influenced by sampling conditions and the biotic and abiotic environment of cells at the time of the analysis (**Fig. 2**).

For both quantitative and qualitative analyses of large datasets, Raman data are often processed with computational algorithms[8,12] (**Fig. 2**). Because interpretation can often depend on the presence of peak shoulders or small changes in peak locations on the order of a few tens of

wavenumbers as is the case in isotope labelling, any computational treatment can potentially affect the interpretation of microbiological Raman data.

Considering these three aspects, microbiological Raman data share similarities to other types of microbiological data, namely those derived from -omics approaches. While fields that rely on the use of these data types have greatly benefitted from the availability of organized central and public repositories for published data with reporting standards, the lack of an actively maintained, open-access data repository for microbiological Raman data has been an obstacle to the wider adoption of Raman spectroscopy in microbiology. Currently, published data are scattered across various sources (e.g., deposited on a journal publication webpage or an author's personal or institutional repository) in the absence of rational and clear reporting standards, making it challenging for researchers to access and use the data. There are several databases commercially available, for example, KnowItAll (https://sciencesolutions.wiley.com/solutions/technique/raman/knowitall-raman-collection/) and one by S.T. Japan Inc. (https://www.stjapan.de/spectra-databases/raman-spectra-databases/). These databases aim to cover the broad range of organic and inorganic materials, and are not specific to microbiological Raman data. As such, considering the peculiarities of microbiological Raman data described above, a database tailored to microbiological Raman data can be highly beneficial to promote sharing and reuse of microbiological Raman data across diverse users within the community. Moreover, in light of how useful research databases like GenBank (https://www.ncbi.nlm.nih.gov/genbank/) and Uniprot (https://www.uniprot.org/) have proven to be, we are witnessing the unique power of 'collective intelligence', where each user plays an important role for data accumulation over time and the amassed data are used for further analyses from different perspectives by other users. Given the similarity of microbiological Raman data to those in these databases, a bottom-up, open-access data repository would significantly reinforce the power and usefulness of Raman spectroscopy in microbiology.

In this context, we announce the establishment of an open-access web-based repository for microbiological Raman data, residing within the BioStudies database[13] maintained by a public institution, the European Bioinformatics Institute (EMBL-EBI). This centralized repository minimizes the risk of data loss or eventual abandonment, offering a long-term common reference for analysis with advantages in accessibility and transparency over commercial data analysis tools. The data collection, called 'MicrobioRaman' (https://www.ebi.ac.uk/biostudies/MicrobioRaman/studies), was inspired by the great success and usefulness of research databases like GenBank and Uniprot, as well as by discussions among the

authors of this Correspondence. The platform is now open for current and future Raman users — covering data from normal Raman spectroscopy to its advanced variant systems[8,14] such as, but not limited to, resonance Raman spectroscopy, stimulated Raman spectroscopy (SRS), coherent anti-Stokes Raman spectroscopy (CARS), surface-enhanced Raman spectroscopy (SERS), tip-enhanced Raman spectroscopy (TERS), hyper Raman spectroscopy (HRS), spatially offset Raman spectroscopy (SORS), polarized Raman spectroscopy, and time-gated (TG) Raman spectroscopy. Step-by-step, recipe-style instructions for deposition of novel datasets are provided on the help page (https://www.ebi.ac.uk/biostudies/submissions/help).

MicrobioRaman aims to provide a comprehensive repository of Raman data acquired from fundamental and applied microbiology research (**Fig. 1b**). The platform was collaboratively developed among the authors of this Correspondence, and it establishes a set of standards for data reporting to ensure reproducible Raman measurements across different users.

The standards for data reporting consist of five sections (**Table 1**): (i) general information about the authors and project underlying novel data submitted; (ii) biological context, including both general information and specific sample details; (iii) experimental conditions, encompassing the setup used for Raman measurements; (iv) data processing, particularly focusing on the treatment of the spectrum; and (v) instrument metadata, such as the type of spike filter, detector specifications, and details of the microscope objective. Additionally, the platform allows data submitters to specify a public release date for newly deposited data, for example, to ensure compliance with publication embargos.

As MicrobioRaman grows, it will become a valuable resource with diverse applications. It will serve as a chemical catalogue, housing data on the distribution of compounds across taxa and ecosystems. Furthermore, it will function as a source of standardised experimental designs, inspiring novel approaches. The current wave of applications of machine learning is already beginning to impact Raman-based approaches in microbiology. The ability to collect Raman data and make them broadly accessible is timely in this regard, as the effectiveness of machine learning approaches often relies on collective intelligence — in particular, data in the repository may be reused as part of training datasets in supervised approaches[8,12].

In conclusion, we believe that, by establishing reporting standards and facilitating data sharing among Raman users, MicrobioRaman will play an important role in promoting the adoption of Raman spectroscopy in microbiology. This initiative represents a cornerstone for reproducible

Raman measurements and will seed further developments in this field. We envision the development of new functions for MicrobioRaman as it grows with active participation from Raman users in the community and the accumulation of novel microbiological Raman data. With this Correspondence, we pledge to deposit our future data into this newly constructed infrastructure and we encourage other Raman users to contribute, further reinforcing the power and potential of reproducible Raman measurements in microbiology.

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Additional information

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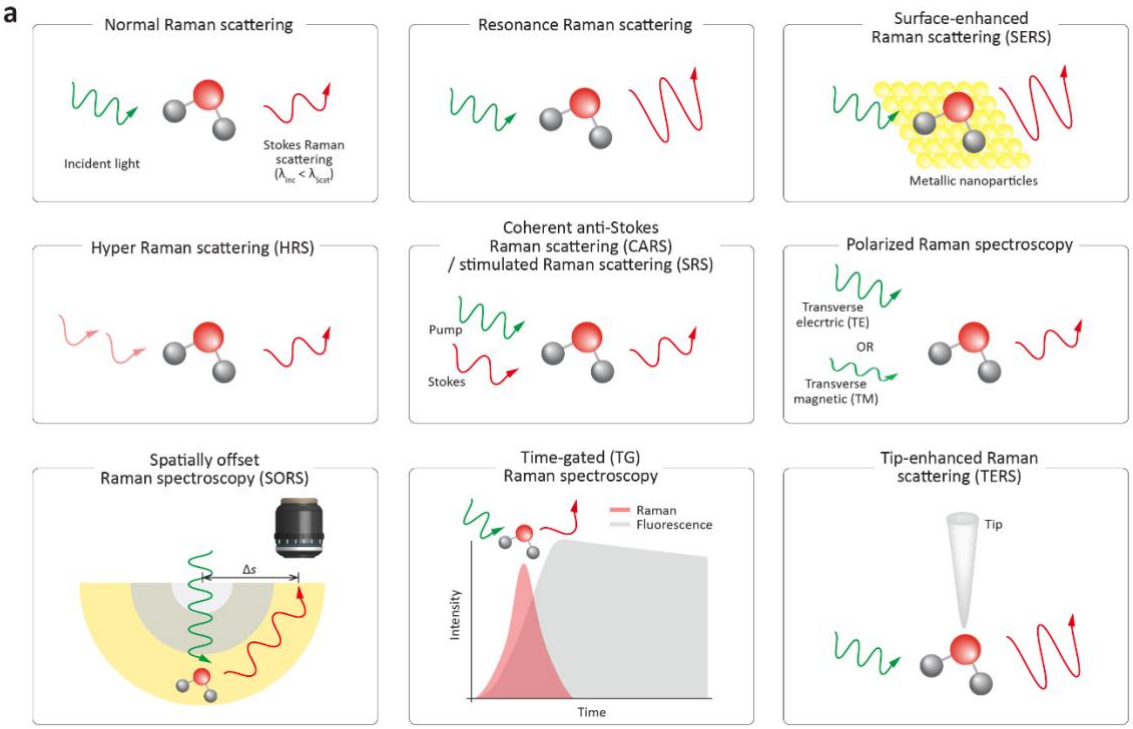
Author contributions

K.S.L., Z.L., A.A., U.S., and R.S. wrote the manuscript. All authors reviewed and approved the manuscript.

Competing interests

The authors declare no competing interests.

Figures


a
Normal Raman scattering
Incident light
Stokes Raman scattering
Resonance Raman scattering
Surface-enhanced Raman scattering (SERS)
Metallic nanoparticles
Hyper Raman scattering (HRS)
Coherent anti-Stokes Raman scattering (CARS) / stimulated Raman scattering (SRS)
Pump
Stokes
Polarized Raman spectroscopy
Transverse elecrtric (TE)
OR
Transverse magnetic (TM)
Spatially offset Raman spectroscopy (SORS)
Δs
Time-gated (TG) Raman spectroscopy
Raman
Fluorescence
Intensity
Time
Tip-enhanced Raman scattering (TERS)
Tip

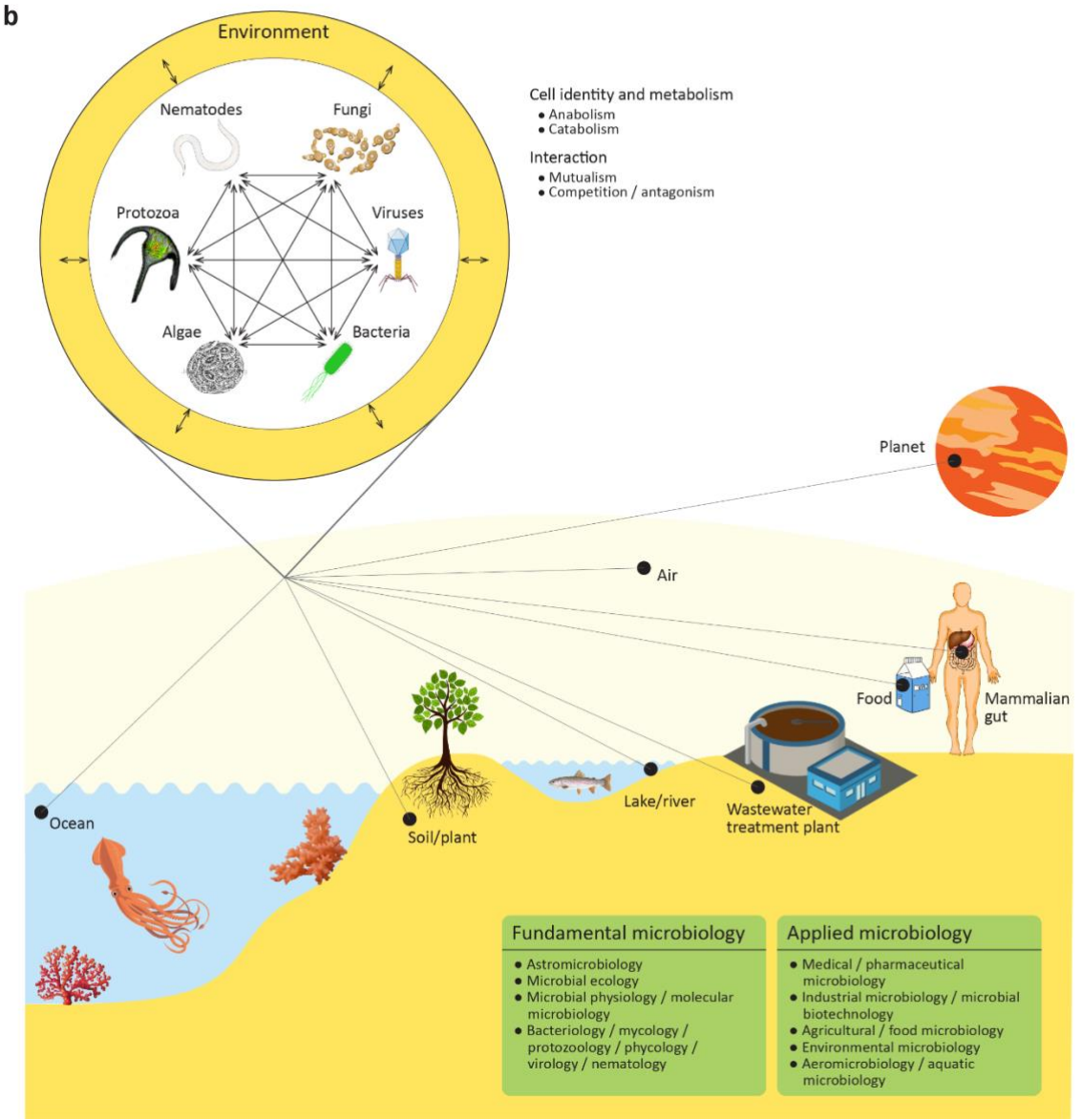

b
Environment
Nematodes
Fungi
Protozoa
Viruses
Algae
Bacteria
Cell identity and metabolism
• Anabolism
• Catabolism
Interaction
• Mutualism
• Competition / antagonism
Planet
Air
Food
Mammalian gut
Ocean
Soil/plant
Lake/river
Wastewater treatment plant
Fundamental microbiology
• Astromicrobiology
• Microbial ecology
• Microbial physiology / molecular microbiology
• Bacteriology / mycology / protozoology / phycology / virology / nematology
Applied microbiology
• Medical / pharmaceutical microbiology
• Industrial microbiology / microbial biotechnology
• Agricultural / food microbiology
• Environmental microbiology
• Aeromicrobiology / aquatic microbiology

Fig. 1 | Overview of Raman technologies and their applications in microbiology. a The working principles underlying normal Raman spectroscopy and its advanced variant systems. For normal Raman spectroscopy, a laser beam interacts with molecules within a sample, resulting in Raman scattering after the interaction. Advanced variant systems, which rely upon modification of the system configuration, can be categorised into three groups depending on their specific advantages: techniques that provide a higher sensitivity for measurement (resonance Raman scattering, surface-enhanced Raman scattering, tip-enhanced Raman scattering), techniques that enable rapid measurement by virtue of the selection of specific wavenumbers (coherent anti-Stokes Raman scattering, stimulated Raman scattering), and techniques that provide other functions, such as the ability to measure peaks not detectable using normal Raman spectroscopy (hyper Raman scattering), among others including spatially offset Raman spectroscopy, polarized Raman spectroscopy, and time-gated Raman spectroscopy. For a more comprehensive presentation of the working principles and system configurations, see refs. [8,15–22]. **b** Applications of Raman spectroscopy in fundamental and applied microbiology. Raman spectroscopy is a versatile technique that enables the measurement of a broad size range of samples across diverse geographical regions — from large nematodes to minuscule viruses found in oceans, soils, mammalian guts, industrial plant systems, and even other planets. By measuring the presence of peaks corresponding to specific macromolecules or differences in spectral shape, peak position, and relative intensity between Raman peaks, often in conjunction with other complementing techniques (e.g., SIP, FISH), Raman spectroscopy facilitates the investigation of microbial diversity in terms of cell identity, metabolism, and functional roles within complex communities and the environment. It also sheds light on the interactions of cells with other cells, their hosts, and the environment. This wide-ranging applicability of Raman spectroscopy makes it an invaluable tool in the field of microbiology.

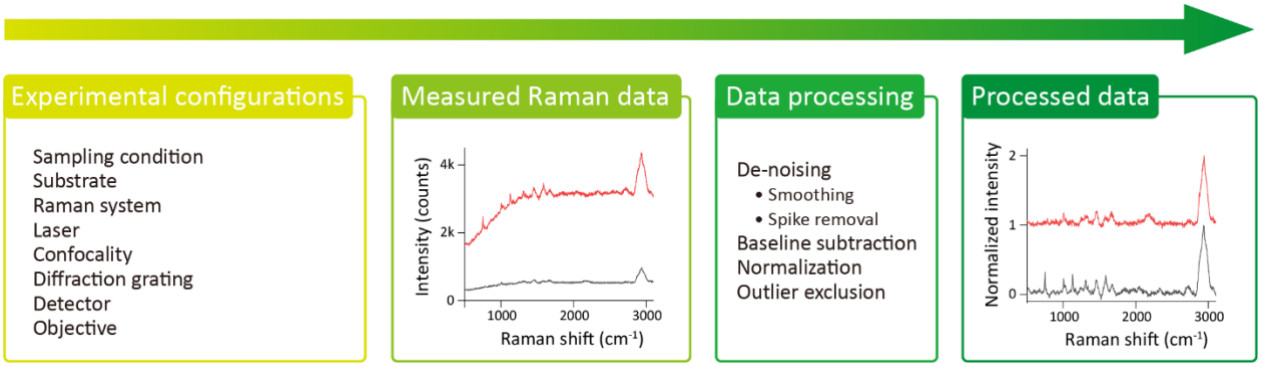


Fig. 2 | Pipeline for measurement and analysis of microbiological Raman data and the parameters that influence the resulting data. Experimental configurations, in addition to the samples themselves, determine the resulting Raman data. When measured Raman spectra display a different level or shape of spectral background, they require computational data processing for quantitative or qualitative analyses and comparisons between samples. A section describing these factors is a part of the reporting standard in the 'MicrobioRaman' repository.

Table 1 | Reporting standards for microbiological Raman data. The 'general' section describes general information about the submission; the 'sample' section provides the biological context and treatment; the 'setup' section provides experimental conditions; the 'treated spectrum' section describes data processing; and the 'instrument metadata' section provides additional instrumental information that could help users to reproduce the measurements. Parameters are colour-coded according to the level of recommended reporting: mandatory (in orange), if applicable (in grey), and recommended (in blue). See also the help page of BioStudies (https://www.ebi.ac.uk/biostudies/submissions/help) for general instructions for submission of novel data.

Section	Parameter	Description
General	Title	Project title
	Release date	Desired release date, for example, to ensure compliance with a publication embargo
	Description	Brief description of the project
	Contacts	Contact details for data authors
	Raw data files	Unprocessed raw Raman data composed of wavenumbers and corresponding Raman intensities
	Publications	Information about associated publications (authors, title, journal name, year)
Sample	Name of cell or compound	Sample names
	Source	Source of a sample, such as a strain collection, a chemical supplier, or the environment or tissue from which a sample was obtained
	Composition	Entities contained in the sample, including not just the cells of interest, but also the medium, as well as any extraneous materials such as tissue, debris, biofilm matrix, or soil
	Sample condition	Whether the cells were dry or wet, fixed or unfixed, and the medium in which they were suspended
	Mounting substrate	E.g., glass coverslip, aluminum slide, CaF_2 slide
	Image files	Image files from Raman imaging
Setup	Raman system	Manufacturer and model of scope
	Measurement type	E.g., normal Raman scattering; resonance Raman scattering; coherent anti-Stokes Raman scattering (CARS); stimulated Raman scattering (SRS); hyper Raman scattering (HRS); surface-enhanced Raman scattering (SERS); spatially offset Raman spectroscopy (SORS); polarized Raman spectroscopy; tip-enhanced Raman scattering (TERS); time-gated (TG) Raman spectroscopy
	Lasers	Wavelength and power of lasers, laser illumination spot diameter, neutral density filter
Treated spectrum	Processed data files	Processed Raman data
	Data treatments	List of computational algorithms and their parameters and sources used for data processing

Instrument metadata	Annotations	E.g., the type of spike filter, detector specifications, details of a microscope objective or focusing lens