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Reporting Summary

Nature Research wishes to improve the reproducibility of the work that we publish. This form provides structure for consistency and transparency in reporting. For further information on Nature Research policies, see our <u>Editorial Policies</u> and the <u>Editorial Policy Checklist</u>.

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For all statistical analyses, confirm that the following items are present in the figure legend, table legend, main text, or Methods section.
n/a Confirmed
\square The exact sample size (<i>n</i>) for each experimental group/condition, given as a discrete number and unit of measurement
A statement on whether measurements were taken from distinct samples or whether the same sample was measured repeatedly
The statistical test(s) used AND whether they are one- or two-sided Only common tests should be described solely by name; describe more complex techniques in the Methods section.
A description of all covariates tested
A description of any assumptions or corrections, such as tests of normality and adjustment for multiple comparisons
A full description of the statistical parameters including central tendency (e.g. means) or other basic estimates (e.g. regression coefficient) AND variation (e.g. standard deviation) or associated estimates of uncertainty (e.g. confidence intervals)
For null hypothesis testing, the test statistic (e.g. <i>F</i> , <i>t</i> , <i>r</i>) with confidence intervals, effect sizes, degrees of freedom and <i>P</i> value noted <i>Give P values as exact values whenever suitable.</i>
For Bayesian analysis, information on the choice of priors and Markov chain Monte Carlo settings
For hierarchical and complex designs, identification of the appropriate level for tests and full reporting of outcomes
\square Estimates of effect sizes (e.g. Cohen's d , Pearson's r), indicating how they were calculated
Our web collection on <u>statistics for biologists</u> contains articles on many of the points above.
Software and code
Policy information about <u>availability of computer code</u>
Data collection The measurmenet software oif the Raman mcirsicopes was used
Data analysis Code was made avalaiabel: https://github.com/Bocklitz-Lab/Example-Raman-spectral-analysis
For manuscripts utilizing custom algorithms or software that are central to the research but not yet described in published literature, software must be made available to editors and reviewers. We strongly encourage code deposition in a community repository (e.g. GitHub). See the Nature Research guidelines for submitting code & software for further information.

Data

Policy information about <u>availability of data</u>

All manuscripts must include a data availability statement. This statement should provide the following information, where applicable:

- Accession codes, unique identifiers, or web links for publicly available datasets
- A list of figures that have associated raw data
- A description of any restrictions on data availability

We provided one of teh datasets as open soure rpositorxy: https://github.com/Bocklitz-Lab/Example-Raman-spectral-analysis

	ne below that is the best fit for your research. If you are not sure, read the appropriate sections before making your selection.
Life sciences	Behavioural & social sciences Ecological, evolutionary & environmental sciences
or a reference copy of t	the document with all sections, see nature.com/documents/nr-reporting-summary-flat.pdf
ife scier	nces study design
-110 30101	ices study design
II studies must dis	sclose on these points even when the disclosure is negative.
Sample size	Published dataset were used to present the protocol.
Data exclusions	We dont excluded data from the 4 published datases.
Replication	No replications was peerfomed.
Randomization	Within the pubslied datasets single spectra of different specimen were utilized.
Blinding	The evaluation was done using cross valdiation appaches, which doesnt work with blinded samples/data.

Materials & experimental systems Methods n/a Involved in the study n/a Involved in the study Antibodies ChIP-seq Eukaryotic cell lines Flow cytometry Palaeontology and archaeology MRI-based neuroimaging Animals and other organisms Human research participants Clinical data Dual use research of concern