SUPPORTING INFORMATION

A manual and an automatic TERS based virus discrimination

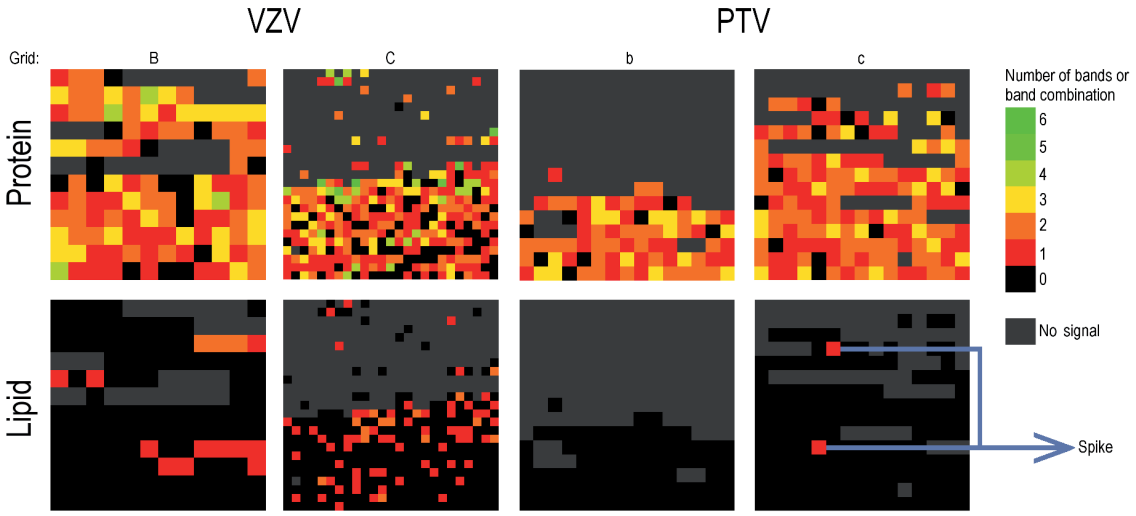
Konstanze Olschewski,[a,b,‡] Evelyn Kämmer,[a,b,c,‡] Stephan Stöckel,[a,b] Thomas Bocklitz,[a,b,c] Tanja Deckert-Gaudig,[c] Roland Zell,[d] Dana Cialla-May,[a,b,c] Karina Weber,[a,b,c] Volker Deckert[a,b,c] and Jürgen Popp[a,b,c,*]

SI-Table S1 Grid parameter

Virus	Grid	Dimension (x×y) [μm]	Points (x×y)	Distance (x×y) [nm]	Numbers of spectra all	manual	automatic
VZV	A	0.10×0.10	12×12	$8.\overline{3}\times8.\overline{3}$	144	78	132
	B	0.15×0.15	12×12	12.5×12.5	144	117	122
	C	0.40×0.40	25×25	16.0×16.0	625	337	548
PTV	a	0.05×0.05	12×12	$4.1\overline{6}\times4.1\overline{6}$	144	128	121
	b	0.06×0.06	15×15	4.0×4.0	225	82	193
	c	0.10×0.10	15×15	$6.\overline{6}\times6.\overline{6}$	225	152	206

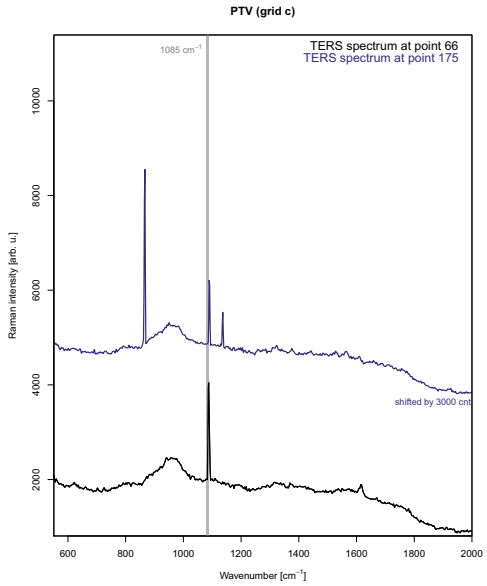
In SI-Tab. S1 the grid dimension of each TERS measurement of VZV and PTV is registered. The lateral dimension is specified in micrometer next to the number of the respective points in the x and y directions as well as the resulting spacing between the individual measuring points in nanometre. The last three columns of the table specify the number of originally measured spectra per grid as well as the number of spectra that remained in the data set for further analysis after the manual and automatic quality rating.

[a] *Institute of Physical Chemistry and Abbe Center of Photonics, Friedrich Schiller University, Helmholtzweg 4, 07743 Jena Germany*
[b] *InfectoGnostics Forschungscampus Jena e.V., Zentrum für Angewandte Forschung, Philosophenweg 7, 07743 Jena, Germany*
[c] *Leibniz Institute of Photonic Technology (IPHT), Albert-Einstein-Strasse 9, 07745 Jena, Germany*
[d] *Department of Virology and Antiviral Therapy, Jena University Hospital, Friedrich Schiller University, Hans-Knöll-Strasse 2, 07745 Jena, Germany*
[‡] *These authors contributed equally to this work*



SI-Figure S1 Component maps for the lipid and protein categories of the two additional virions of VZV (left, map: B & C) as well as the two of PTV (right, map: b & c).

In SI-Fig. S1 component maps of both categories for two additional virions of VZV and PTV are illustrated. The respective grid dimensions can be found in SI-Tab. S1. In addition to the component map in Fig. 3, the different lipid content of VZV and PTV is evidently shown. The PTV viruses exhibit no lipid components in their structure. However, in the map c two points bear a lipid signal. Upon closer examination of the corresponding spectra, spikes show up in the expected wavenumber range of the phospholipid. These spikes cause false positive values in the lipid component map c of the PTV. The two relevant spectra are shown in SI-Fig. S2. An automatic spike removal was omitted in this study because of the very similar appearance of the spikes and the peaks. Using the available device, spikes showed a relatively large bandwidth whereas some of the Raman signals were intense and sharp. The last mentioned arises through an optimal alignment between TERS tip and molecule. This complicated the spike removal with common algorithms. The signal loss was higher than the improvement obtained by a spike removal attempt. Therefore, spikes remained in the used data.



SI-Figure S2 TERS spectra of grid c measured on a *Porcine teschovirus*. The spikes in both spectra (number: 66 & 175) located in the range of interest for the phospholipid band (labelled in grey) cause false positive values in the component map of the lipid category (see SI-Fig. S1).