Electronic Supplementary Material (ESI) for Analyst.

Supporting Information:

Towards therapeutic drug monitoring of antibiotic level - analyzing pharmacokinetics of levofloxacin by using DUV-resonance Raman spectroscopy

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Supplementary Material

Figure S1

Exemplary workflow of data evaluation. First, the untreated Raman spectra (A) of water (orange, 1), 20 and 50 µM levofloxacin (2 and 3) were scatter corrected ***via*** the EMSC algorithm (B). Then, for quantification, the respective difference spectra were calculated using the water spectrum as a reference and the Raman signal at about 1400 cm^{-1} was investigated.

Figure S2

Alignment of the experimental FT Raman spectrum of levofloxacin (1) with the calculated scattering activities (calculation method: B3LYP/cc-pVTZ) and their Gaussian peak profile (FWHM = 20 cm^{-1}, 2). The scaling factor and the resulting MAE value for the investigated wavenumber region (1800-200 cm^{-1}) are 0.98 and 1.41, respectively.

Figure S1

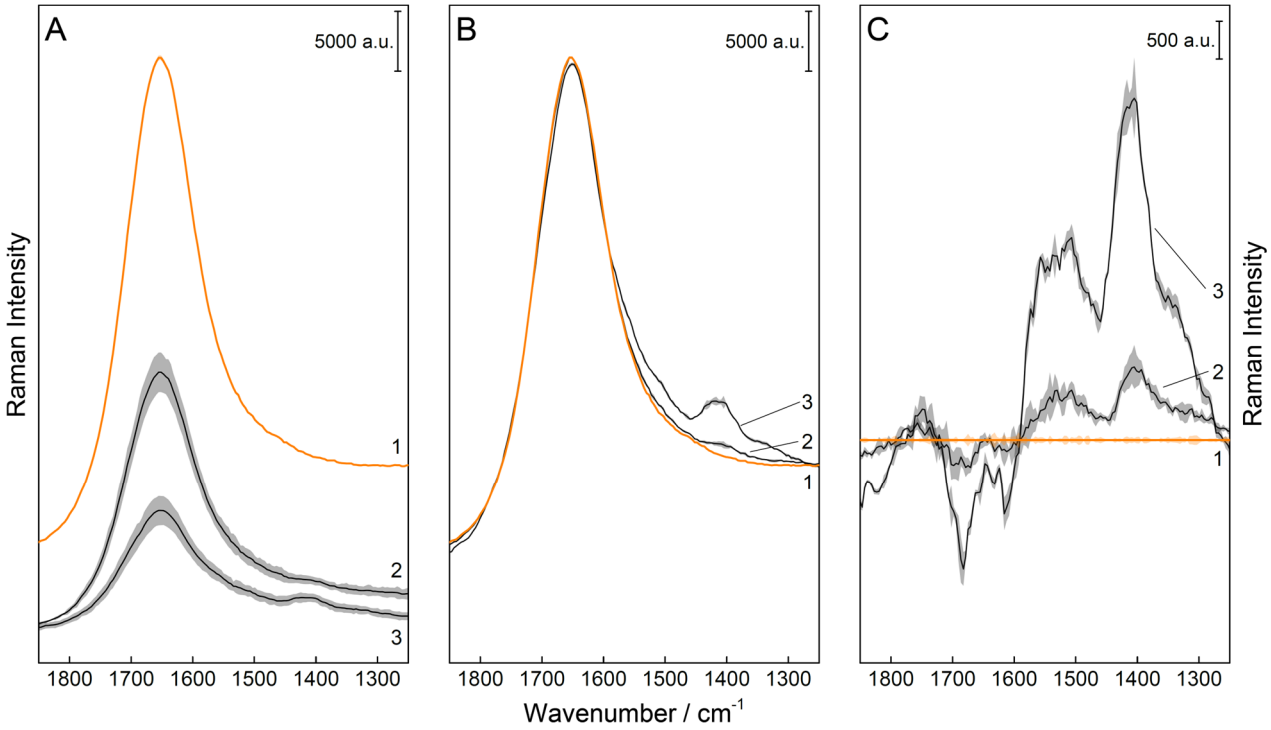

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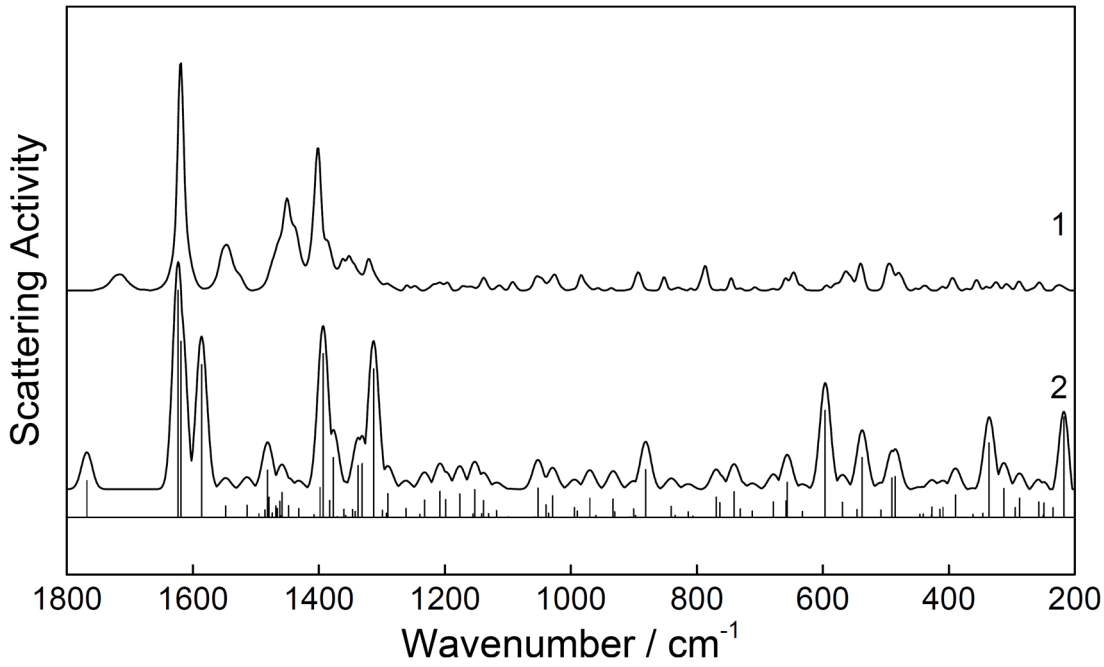
Figure S2



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