Supplementary Material

Fiber enhanced Raman spectroscopic analysis as a novel method for diagnosis and monitoring of diseases related to hyperbilirubinemia and hyperbiliverdinemia

Di Yan¹, Christian Domes¹, Robert Domes¹, Timea Frosch¹, Jürgen Popp¹,³,⁴, Mathias W. Pletz², Torsten Frosch¹,³,⁴,*

¹Leibniz Institute of Photonic Technology, Jena, Germany
²University Hospital, Center for Infectious Diseases and Infection Control, Jena, Germany
³Friedrich Schiller University, Institute for Physical Chemistry, Jena, Germany
⁴Friedrich Schiller University, Abbe Centre of Photonics, Jena, Germany
*corresponding author: torsten.frosch@uni-jena.de, torsten.frosch@gmx.de

**Figure S1**
Comparison of the experimental FT-Raman spectra (λexc. = 1064 nm) of bilirubin (A1) and biliverdin (B1) with the calculated Raman spectra (B3LYP/cc-pVTZ) of bilirubin (in water (PCM): A2 and in gas phase: A3) and biliverdin (in water (PCM): B2 and in gas phase: B3). The scaling factors for A were 0.9762 and 0.9809 and for B were 0.9794 and 0.9792 for the gas phase and the PCM calculation, respectively.
Figure S2
Raman spectra of 100 µM bilirubin (A), 1 µM biliverdin (B), and their mixture (C) with λexc = 364 nm.