SUPPLEMENTARY INFORMATION

Non-invasive Depth Determination of Inclusion in Biological Tissues using Spatially Offset Raman Spectroscopy with External Calibration

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SI1 – Schematic of the experimental set-up and samples

SI2 – Results of Monte Carlo modelling (mean path length, ratio, standard error)

SI3 – Calibration model based on different SF, RMSEP of different model

SI1: (A) Schematic of the experimental set-up described in the material and method section. (B) Schematic diagram of the model samples: layered turbid media (grey); inclusion (blue cylinder)
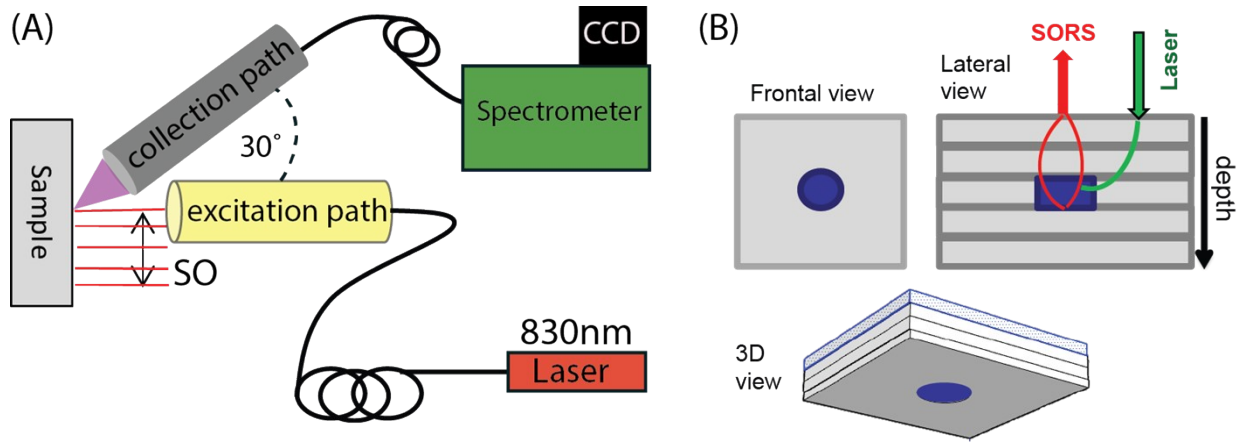
SI2: Monte Carlo modelling: Mean path length resulting for different pair of optical properties (μ_a and μ_s') of the two geometry (mp_{SORS} and mp_{DEPTH}) with the relative standard deviation (σ). Scaling factor SF calculated as ratio of two mean path length.

µa(mm⁻¹)	µs'(mm⁻¹)	mp$_{SORS}$	mp$_{DEPTH}$	σ(mp$_{SORS}$)	σ(mp$_{DEPTH}$)	SF - RATIO	σ (SF)
0	0.5	143.2	58.5	0.22	0.02	**2.45**	0.19
0	1	240.0	82.2	1.03	0.02	**2.92**	0.81
0	1.5	307.5	127.7	1.40	0.03	**2.41**	1.04
0	2	311.5	155.0	1.90	0.07	**2.01**	1.36
0.005	0.5	116.0	39.0	0.70	0.02	**2.97**	0.56
0.005	1	257.2	83.6	1.50	0.03	**3.08**	1.19
0.005	1.5	306.0	124.0	0.44	0.03	**2.47**	0.36
0.005	2	342.0	154.0	1.40	0.04	**2.22**	1.03
0.01	0.5	121.0	45.0	0.40	0.04	**2.69**	0.37
0.01	1	243.0	101.7	0.94	0.10	**2.39**	0.83
0.01	1.5	308.0	127.3	1.80	0.06	**2.42**	1.38
0.01	2	354.0	153.6	2.20	0.06	**2.30**	1.63
0.05	0.5	131.0	50.0	0.20	0.02	**2.62**	0.18
0.05	1	243.6	94.0	1.00	0.04	**2.59**	0.80
0.05	1.5	326.0	130.2	1.60	0.06	**2.50**	1.25
0.05	2	332.0	163.0	2.60	0.07	**2.04**	1.84
0.1	0.5	145.0	57.7	0.22	0.01	**2.51**	0.18
0.1	1	230.0	102.0	1.10	0.03	**2.25**	0.81
0.1	1.5	333.5	136.9	1.50	0.07	**2.44**	1.18
0.1	2	330.4	159.8	2.40	0.07	**2.07**	1.72

SI3: Different calibration models for depth prediction of SERS NPs in ex-vivo tissues. (a) Comparison of internal calibration (black dot and line), external calibration with SF= 2.61 (red dot and line) resulting from MC calculation for $\mu_s' = 0.5$ mm^{-1} $\mu_a = 0.05$ mm^{-1} , external calibration with the average SF= 2.46 resulting from all MC calculation with pair of values of μ_a = (0, 0.005, 0.01, 0.05, 0.1) mm^{-1} and μ_s' = (0.5, 1, 1.5, 2) mm^{-1} (b) RMSEP of different models.

(a)

(b)