Supplementary Information

Material-Agnostic Characterization of Spatially Offset Raman Spectroscopy in Turbid Media via Monte Carlo Simulations

Zuriel Erikson Joven^a, Piyush Raj^a, and Ishan Barman^{* a,b,c}

- a) Department of Mechanical Engineering, Johns Hopkins University, Baltimore, Maryland 21218, United States of America
- b) Department of Oncology, Johns Hopkins University, Baltimore, Maryland 21287, United States of America
- c) The Russell H. Morgan Department of Radiology and Radiological Science, The Johns Hopkins University, School of Medicine, Baltimore, Maryland 21205, United States of America



Figure S1. Maximum attainable SNR_{photon} values and corresponding δ_{opt} and ζ_{opt} values follow similar dependencies on *D* and *z* in different materials. Representative SNR_{photon} versus ζ plots at z = 0.5 cm (i) and 1.5 cm (ii) and $\delta = 0.2, 0.5, 1.0$ cm, $\max_{\zeta}(SNR_{photon})$ versus δ plots at z = 0.5 cm (iii) and 1.5 cm (iv), $\max_{\delta,\zeta}(SNR_{photon})$ versus (*D*, *z*) log-scale plots (v), δ_{opt} versus (*D*, *z*) plots (vi), and ζ_{opt} versus (*D*, *z*) plots (vii) for $\mu_s = 10$ cm⁻¹ (A) and $\mu_s = 100$ cm⁻¹, $\mu_a = 1$ cm⁻¹ (B).



Figure S2. Visual representation of collected Raman intensity, η , in log-scale, along a twodimensional slice coplanar to the excitation (orange arrow) and collection (red arrow) probes, at $\delta = 0.2 \text{ cm}$ (i), $\delta = 0.5 \text{ cm}$ (ii) and $\delta = 1.0 \text{ cm}$ (iii), for $\mu_s = 10 \text{ cm}^{-1} \& \mu_a = 0.1 \text{ cm}^{-1}$ (A), $\mu_s = 10 \text{ cm}^{-1}$ $\& \mu_a = 1.0 \text{ cm}^{-1}$ (B), $\mu_s = 100 \text{ cm}^{-1} \& \mu_a = 0.1 \text{ cm}^{-1}$ (C), and $\mu_s = 100 \text{ cm}^{-1} \& \mu_a = 1.0 \text{ cm}^{-1}$ (D).

Figure S2 shows that large values of η follow a curved subsurface path, with hotspots close to either the laser or detector. In some cases, η is clearly greater at the laser than at the detector (Figure 2A-C.ii-iii). The raw data and Monte Carlo code used to obtain the various η distributions in this study are available on Github: <u>https://github.com/zurieljoven/SORS-Simulations/</u>