

Leonardo C. Pacheco-Londoño¹

Ailee. Y. Chang² and Antonio. Acosta-Hoyo¹

¹ Life Science Research Center (CICV), Universidad Simón Bolívar, Barranquilla, Colombia. ² George Washington University, Washington DC, USA.

leonardo.pacheco@unisimon.edu.co

Two chemical windows on dengue: non-overlapping Raman and SERS signatures under a common chemometric protocol

During early dengue, clinical manifestations can be nonspecific and resemble other febrile infections, complicating diagnosis. Comparing label-free Raman approaches therefore requires a consistent chemometric workflow. We analyzed three dengue datasets using a unified patient-level protocol: (i) conventional Raman spectroscopy of 5 μ L serum droplets at 785 nm (65 dengue, 130 controls) [1]; (ii) AgNP-SERS at 830 nm in an independent cohort (52 dengue, 30 healthy controls, 13 chikungunya); and (iii) AuNP-SERS at 785 nm using 58 patients from the first cohort (35 RT-PCR-positive, 23 RT-PCR-negative/serology-positive). Each participant contributed one independent observation; model selection was confined to the training set, and PLS-DA performance was evaluated over 100 repeated stratified splits.

All five models showed comparable performance (Figure 1), with sensitivities of 0.81–0.87 and specificities of 0.88–0.96. In matched samples at 785 nm, conventional Raman distinguished RT-PCR-positive cases from RT-PCR-negative patients and controls with 0.84 sensitivity and 0.96 specificity [1], whereas AuNP-SERS separated RT-PCR-positive from RT-PCR-negative patients with 0.87 sensitivity and 0.88 specificity. This AuNP-SERS result should be considered an upper-bound estimate because classes were acquired in separate sessions.

Despite similar performance, discriminant bands showed little overlap. Conventional Raman highlighted 557, 616, 1028, 1446, and 1525 cm^{-1} , with additional viremia-related contributions near 1289 and 1080–1120 cm^{-1} . AgNP-SERS emphasized 478, 725, 1009, 1133, and 1400 cm^{-1} , particularly the purine-associated 725 cm^{-1} band [3]. AuNP-SERS identified viremia mainly through 728, 1000, and 1540 cm^{-1} , with only partial overlap around 616–640 cm^{-1} . Thus, Raman and SERS achieved comparable classification through distinct molecular signatures. The matched-sample comparison indicates that this divergence is driven mainly by platform chemistry rather than cohort differences, supporting their complementary use for molecular characterization of dengue. These complementary spectral windows may therefore provide broader biochemical information than either platform alone and strengthen multimodal strategies for dengue detection and viremia assessment clinically.

References

- [1] Guerra-Simanca, L., et al. (2026). *Dengue Screening and Viremia Stratification by Raman Spectroscopy of Serum Liquid Biopsies*. ACS Omega. Manuscript ID: ao-2026-051943.R1. Revised manuscript submitted after peer review; under editorial review.

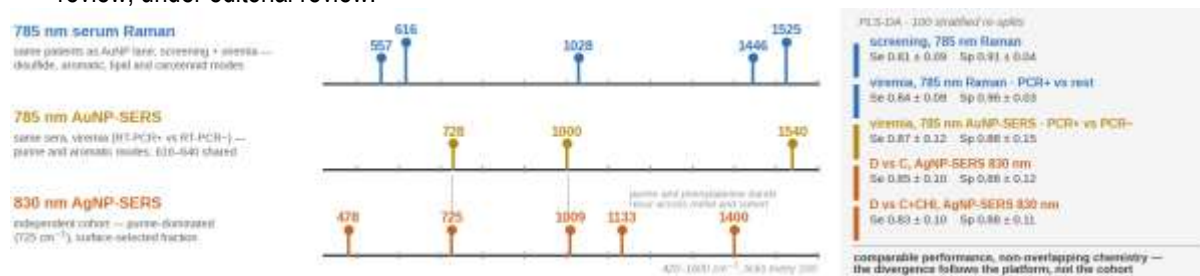


Figure 1: Highest-ranked PLS-DA VIP positions of the three regimes (axis 420–1600 cm^{-1} , ticks every 100) and re-split performance; the two 785 nm lanes share the same patients; dotted guides mark the purine and phenylalanine bands shared by both SERS sets.