Electronic Supplementary Material (ESI) for Journal of Materials Chemistry B

Rapid detection of oral cancer using Ag-TiO_2 nanostructured surface-enhanced Raman spectroscopic substrates

Chundayil Madathil Girish, [a] Subramania Iyer, [b] Krishnakumar Thankappan, [b] V. V. Divya Rani, [a] G. Siddaramana Gowd, [a] Deepthy Menon, [a] Shantikumar Nair, [a] Manzoor Koyakutty*[a]

[a]*Amrita Centre for Nanosciences & Molecular Medicine, Amrita Vishwa Vidyapeetham University, Cochin, India- 682041*

[b]*Department of Head and Neck Surgery, Amrita Institute of Medical Sciences, Cochin, India- 682041*

SUPPORTING INFORMATION

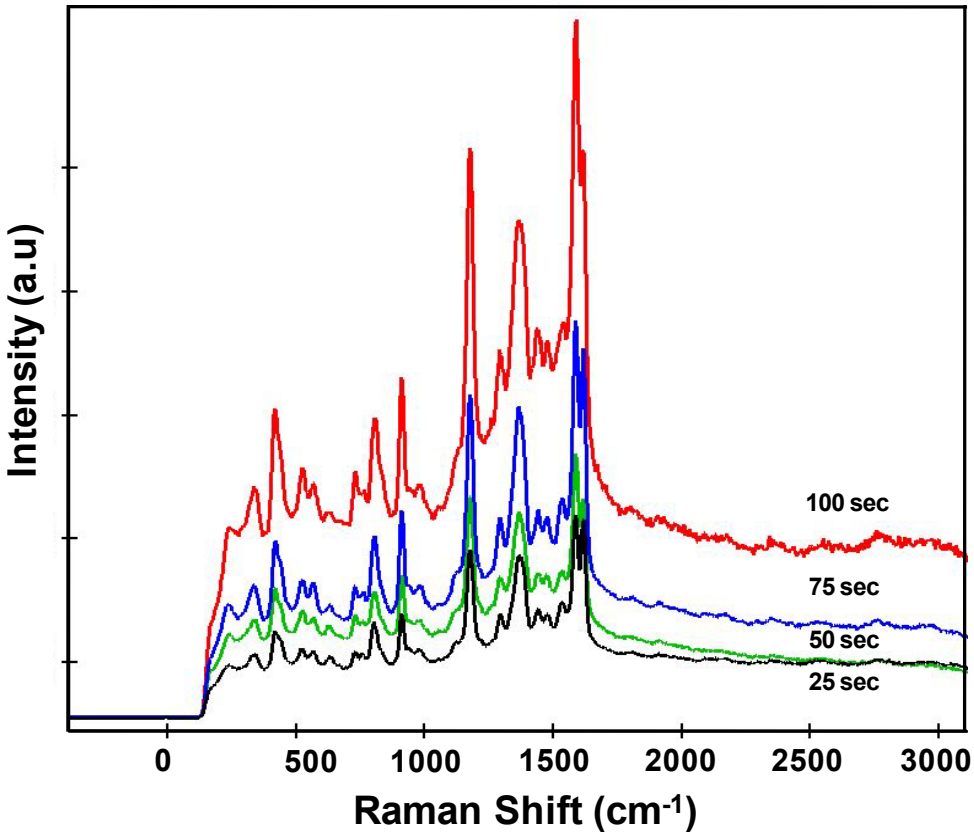

Fig. S1: SERS spectrum of CV (10 μM) obtained from NB substrates coated with Ag at various sputtering conditions (40 mA) for time duration of 25, 50, 75 and 100 s (Integration time: 0.5 s, Accumulations: 10)

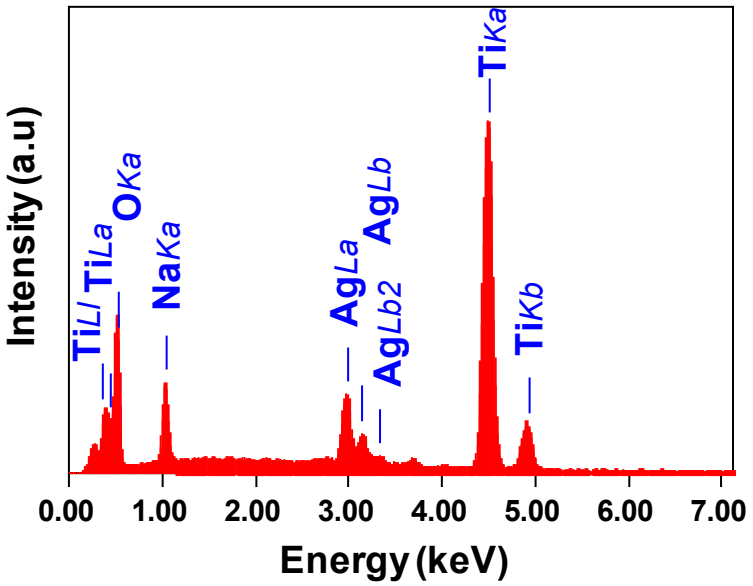

Fig. S2: the EDS pattern of NL after Ag sputter deposition at 40 mA for 100 s (Ti- Titanium, Au- Gold, Ag- silver, O- Oxygen, Na- Sodium).

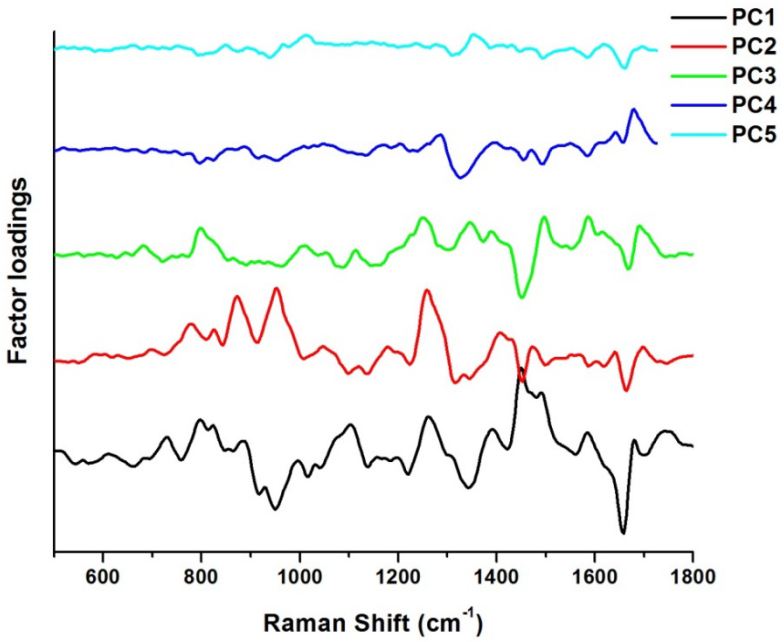

Fig. S3: Spectral loadings of five most diagnostically significant PCs.

A:

Observation	Prior	Posterior	Normal	Tumor
Obs1	Normal	Normal	1.000	0.000
Obs2	Normal	Normal	1.000	0.000
Obs3	Normal	Normal	1.000	0.000
Obs4	Normal	Normal	1.000	0.000
Obs5	Normal	Normal	1.000	0.000
Obs6	Normal	Normal	1.000	0.000
Obs7	Tumor	Tumor	0.000	1.000
Obs8	Tumor	Tumor	0.000	1.000
Obs9	Tumor	Tumor	0.000	1.000
Obs10	Tumor	Tumor	0.000	1.000
Obs11	Tumor	Tumor	0.000	1.000
Obs12	Tumor	Tumor	0.000	1.000
Obs13	Normal	Normal	1.000	0.000
Obs14	Normal	Normal	1.000	0.000
Obs15	Normal	Normal	1.000	0.000
Obs16	Normal	Normal	1.000	0.000
Obs17	Normal	Normal	1.000	0.000
Obs18	Normal	Normal	1.000	0.000
Obs19	Tumor	Tumor	0.000	1.000
Obs20	Tumor	Tumor	0.000	1.000
Obs21	Tumor	Tumor	0.000	1.000
Obs22	Tumor	Tumor	0.000	1.000
Obs23	Tumor	Tumor	0.000	1.000
Obs24	Tumor	Tumor	0.000	1.000
Obs25	Normal	Normal	1.000	0.000
Obs26	Normal	Normal	1.000	0.000
Obs27	Normal	Normal	1.000	0.000
Obs28	Normal	Normal	0.657	0.343
Obs29	Normal	Normal	1.000	0.000
Obs30	Normal	Normal	1.000	0.000
Obs31	Tumor	Tumor	0.000	1.000
Obs32	Tumor	Tumor	0.000	1.000
Obs33	Tumor	Tumor	0.000	1.000
Obs34	Tumor	Tumor	0.000	1.000
Obs35	Tumor	Tumor	0.000	1.000
Obs36	Tumor	Tumor	0.000	1.000
Obs37	Normal	Normal	0.641	0.359
Obs38	Normal	**Tumor**	0.375	0.625
Obs39	Normal	Normal	1.000	0.000

Obs40	Normal	Normal	1.000	0.000
Obs41	Normal	Normal	1.000	0.000
Obs42	Normal	Normal	1.000	0.000
Obs43	Tumor	Tumor	0.000	1.000
Obs44	Tumor	Tumor	0.000	1.000
Obs45	Tumor	Tumor	0.000	1.000
Obs46	Tumor	Tumor	0.000	1.000
Obs47	Tumor	Tumor	0.000	1.000
Obs48	Tumor	Tumor	0.000	1.000
Obs49	Tumor	Tumor	0.000	1.000
Obs50	Tumor	Tumor	0.000	1.000
Obs51	Tumor	Tumor	0.000	1.000
Obs52	Tumor	Tumor	0.000	1.000
Obs53	Tumor	Tumor	0.000	1.000
Obs54	Tumor	Tumor	0.000	1.000
Obs55	Tumor	Tumor	0.000	1.000
Obs56	Tumor	Tumor	0.000	1.000

B:

from \ to	Normal	Tumor	Total	% correct
Normal	23	1	24	95.83%
Tumor	0	32	32	100.00%
Total	23	33	56	98.21%

Table 1: (A) Cross-validation results of DA showing prior and posterior classification, membership probabilities of each individual spectrum. One spectrum taken from normal tissue (Obs 38) was classified as tumor by DA whereas all other spectrum were classified correctly to their respective groups (B) Confusion matrix for the cross-validation results showing the specificity, sensitivity and accuracy of classification as 95.83%, 100% and 98.21%, respectively.