

Supplementary information

Label-free blood plasma test based on surface-enhanced Raman scattering for tumor stages detection in nasopharyngeal cancer

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Table S1. Clinical information on nasopharyngeal cancer patients

No.	Age	Sex	T stage	Pathological type	VCA-IgA (s/co)	EA-IgA (s/co)	EBV-DNA (copies/ml)
1	44	male	T1	non cornification undifferentiated carcinoma	4.05	2.02	5.59×10^2
2	65	male	T1	Poorly differentiated squamous cell carcinomas	1.78	0.67	6.21×10^2
3	52	male	T1	non cornification undifferentiated carcinoma	2.96	0.94	
4	45	male	T1	Poorly differentiated squamous cell carcinomas	4.33	0.33	5.79×10^2
5	47	male	T1	non cornification undifferentiated carcinoma	2.43	0.32	3.21×10^3
6	49	male	T1	non cornification undifferentiated carcinoma	4.33	1.79	3.60×10^2
7	75	female	T1	vesicular nucleus cell carcinoma	0.55	0.12	1.15×10^2
8	60	male	T1	non cornification undifferentiated carcinoma	4.33	3.88	
9	35	female	T1	squamous cell carcinomas	6.07	1.5	1.29×10^3
10	49	male	T1	non cornification undifferentiated carcinoma	1.16	0.25	$<5.0 \times 10^2$
11	48	male	T1	non cornification undifferentiated carcinoma	2.09	0.19	2.53×10^2
12	46	female	T1	Poorly differentiated squamous cell carcinomas	2.74	0.5	2.85×10^2
13	37	male	T1	non cornification undifferentiated carcinoma	2.28	0.13	8.93×10^2
14	43	female	T1	non cornification undifferentiated carcinoma	4.62	4.44	1.11×10^2
15	71	male	T1	non cornification undifferentiated carcinoma	5.51	4.45	1.07×10^3
16	43	male	T1	non cornification undifferentiated carcinoma	0.17	0.75	1.86×10^3
17	50	female	T1	non cornification	3.83	1.44	$<5.0 \times 10^2$

				undifferentiated carcinoma			
18	56	male	T1	non cornification undifferentiated carcinoma	0.92	0.32	$<5.0 \times 10^2$
19	39	male	T1	non cornification undifferentiated carcinoma	4.55	2.47	1.33×10^3
20	48	male	T1	non cornification undifferentiated carcinoma	3.77	3.8	1.27×10^3
21	37	male	T1	non cornification undifferentiated carcinoma	4.27	2.94	
22	45	male	T1	non cornification undifferentiated carcinoma	2.12	0.45	1.23×10^3
23	43	male	T1	non cornification undifferentiated carcinoma	3.11	1.01	2.27×10^3
24	50	female	T1	non cornification undifferentiated carcinoma	2.09	0.66	1.03×10^3
25	52	male	T1	non cornification undifferentiated carcinoma	1.11	0.45	1.53×10^2
26	45	male	T4	non cornification undifferentiated carcinoma			7.23×10^2
27	42	male	T3	non cornification differentiated carcinoma	2.01	0.27	1.53×10^2
28	44	male	T3	non cornification undifferentiated carcinoma	5.19	4.84	$<5.0 \times 10^2$
29	36	male	T2	non cornification undifferentiated carcinoma	3.47	0.33	$<5.0 \times 10^2$
30	57	female	T3	non cornification undifferentiated carcinoma	1.82	0.37	5.10×10^2
31	65	male	T4	non cornification undifferentiated carcinoma	0.91	0.22	2.19×10^2
32	38	male	T2	non cornification undifferentiated carcinoma	2.65	0.1	$<5.0 \times 10^2$
33	53	female	T4	non cornification undifferentiated carcinoma	4.79	3.79	9.83×10^3
34	52	male	T4	cornification squamous cell carcinomas	2.67	2.17	$<5.0 \times 10^2$
35	52	male	T2	non cornification undifferentiated carcinoma	5.63	1.7	5.07×10^2
36	56	male	T4	non cornification undifferentiated carcinoma	2.6	0.73	1.16×10^4
37	40	male	T2	non cornification undifferentiated carcinoma	6.31	1.78	2.68×10^3
38	62	male	T2	non cornification undifferentiated carcinoma	3.9	1.2	$<5.0 \times 10^2$

39	38	male	T3	non cornification undifferentiated carcinoma	0.65	0.25	1.73×10^3
40	41	male	T4	non cornification undifferentiated carcinoma	1.9	0.15	2.95×10^3
41	36	male	T2	non cornification differentiated carcinoma	4.66	5.13	1.57×10^4
42	61	female	T4	non cornification undifferentiated carcinoma	1.79	0.42	3.71×10^3
43	42	male	T4	Poorly differentiated squamous cell carcinomas	1.09	1	5.0×10^2
44	44	male	T4	non cornification undifferentiated carcinoma	1.54	0.22	1.84×10^3
45	73	female	T4	non cornification undifferentiated carcinoma	3.9	0.13	$<5.0 \times 10^2$
46	69	male	T3	Poorly differentiated squamous cell carcinomas	4.96	2.56	$<5.0 \times 10^2$
47	25	male	T4	non cornification undifferentiated carcinoma	3.8	0.22	$<5.0 \times 10^2$
48	45	male	T3	non cornification undifferentiated carcinoma	4.81	5.82	$<5.0 \times 10^2$
49	47	male	T4	non cornification carcinoma	1.54	5.43	1.15×10^4
50	42	male	T2	non cornification undifferentiated carcinoma	4.37	0.55	1.1×10^3
51	43	male	T4	non cornification carcinoma	5.48	1.13	$<5.0 \times 10^2$
52	55	male	T4	non cornification squamous cell carcinomas	1.44	0.41	1.5×10^1
53	39	male	T2	non cornification undifferentiated carcinoma	2.06	0.49	$<5.0 \times 10^2$
54	65	male	T4	non cornification undifferentiated carcinoma	2.32	0.76	2.01×10^4
55	40	male	T4	non cornification undifferentiated carcinoma	3.07	2.89	1.16×10^3
56	50	male	T3	non cornification undifferentiated carcinoma	7.24	5.41	2.47×10^2
57	57	male	T4	Poorly differentiated squamous cell carcinomas	0.69	0.1	$<5.0 \times 10^2$
58	42	female	T4	non cornification undifferentiated carcinoma	5.62	2.27	1.49×10^2
59	35	female	T3	non cornification undifferentiated carcinoma	7.24	5.4	$<5.0 \times 10^2$
60	52	female	T3	non cornification undifferentiated carcinoma	2.35	0.11	2.19×10^4

61	37	male	T3	non cornification undifferentiated carcinoma	5.33	0.16	1.93×10^4
62	22	female	T2	non cornification undifferentiated carcinoma	7.24	1.84	1.37×10^2
63	54	male	T4	cornification squamous cell carcinomas	6.28	5.41	2.68×10^4
64	26	male	T2	non cornification undifferentiated carcinoma	4.86	0.98	3.28×10^3
65	68	female	T4	non cornification undifferentiated carcinoma	5.48	4.05	1.23×10^3
66	59	male	T2	non cornification carcinoma	4.25	0.58	
67	43	male	T3	non cornification undifferentiated carcinoma	1.38	0.185	2.01×10^5
68	36	female	T3	non cornification undifferentiated carcinoma	1.2	0.09	
69	54	male	T3	non cornification undifferentiated carcinoma	7.25	5.06	1.96×10^3
70	66	male	T3	non cornification carcinoma	5.01	0.86	3.00×10^3
71	57	male	T4	non cornification undifferentiated carcinoma	5.64	0.76	1.06×10^2
72	34	male	T2	non cornification undifferentiated carcinoma	5.9	3.24	$<5.0 \times 10^2$
73	22	male	T3	non cornification undifferentiated carcinoma			
74	59	male	T3	non cornification undifferentiated carcinoma	5.91	0.11	7.91×10^2
75	58	male	T4	non cornification undifferentiated carcinoma	3.05	2.01	$<5.0 \times 10^2$
76	55	male	T4	non cornification undifferentiated carcinoma	4.82	2.66	1.12×10^2
77	66	male	T3	non cornification differentiated carcinoma	1.58	2.89	$<5.0 \times 10^2$
78	51	male	T4	non cornification differentiated carcinoma	2.74	3.06	2.40×10^4
79	46	male	T2	non cornification undifferentiated carcinoma	1.94	0.14	$<5.0 \times 10^2$
80	37	female	T2	non cornification undifferentiated carcinoma	4.39	2.88	$<5.0 \times 10^2$
81	59	male	T4	Poorly differentiated squamous cell carcinomas	5.81	0.69	1.39×10^2
82	54	female	T4	non cornification undifferentiated carcinoma	3.5	0.23	$<5.0 \times 10^2$

83	32	male	T2	non cornification undifferentiated carcinoma	4.716	0.255	$<5.0 \times 10^2$
84	60	male	T3	non cornification undifferentiated carcinoma	6.47	4.83	$<5.0 \times 10^2$
85	74	male	T4	non cornification undifferentiated carcinoma	0.92	0.15	$<5.0 \times 10^2$
86	57	male	T3	Poorly differentiated squamous cell carcinomas	3.09	3.84	4.83×10^3
87	39	female	T3	non cornification undifferentiated carcinoma	4.75	0.57	4.02×10^2
88	65	male	T2	non cornification carcinoma	2.93	0.35	4.27×10^3
89	42	male	T4	non cornification differentiated carcinoma	<0.8	<0.8	$<5.0 \times 10^2$
90	60	male	T2	non cornification differentiated carcinoma			8.98×10^2
91	42	female	T4	non cornification differentiated carcinoma	4.23	<0.8	8.54×10^2
92	15	male	T4	non cornification differentiated carcinoma	5.38	4.02	$<5.0 \times 10^2$
93	59	male	T4	non cornification differentiated carcinoma	2.83	0.47	$<5.0 \times 10^2$
94	27	male	T2	non cornification differentiated carcinoma	1.49	0.13	$<5.0 \times 10^2$
95	64	female	T4	non cornification differentiated carcinoma	7.25	3	2.28×10^5
96	43	female	T3	non cornification undifferentiated carcinoma			
97	34	male	T2	non cornification undifferentiated carcinoma	3.91	3.56	
98	67	male	T2	non cornification undifferentiated carcinoma	3.91	0.67	9.10×10^2
99	43	male	T3	non cornification undifferentiated carcinoma	1.78	0.16	$<5.0 \times 10^2$
100	57	male	T3	non cornification undifferentiated carcinoma	1.6	0.77	8.10×10^2

Table S2. Classification results of blood SERS prediction of the three pathology groups using SERS peak intensity.

Peak (cm ⁻¹)	Diagnostic combinations			Predicted parameters		
				Sensitivity	Specificity	AUC
492	T1	vs.	N	68%	68.3%	0.757
	T2-T4	vs.	N	65.3%	68.3%	0.738
725	T1	vs.	N	88%	63.3%	0.811
	T2-T4	vs.	N	64%	60%	0.688
1003	T1	vs.	N	88%	85%	0.938
	T2-T4	vs.	N	84%	85%	0.909
1068	T1	vs.	N	64%	61.7%	0.646
	T2-T4	vs.	N	72%	75%	0.790
1131	T1	vs.	T2-T4	68%	65.3%	0.658
	T1	vs.	N	84%	73.3%	0.800
	T2-T4	vs.	N	73.3%	76.7%	0.803
1208	T1	vs.	N	76%	76.7%	0.801
	T2-T4	vs.	N	84%	76.7%	0.862
1402	T2-T4	vs.	N	77.3%	75%	0.839
	T1	vs.	T2-T4	69.3%	72%	0.725
1655	T2-T4	vs.	N	73.3%	81.7%	0.839

T1: Tumor 1 stage nasopharyngeal cancer subject; T2-T4: Tumor 2-4 stage nasopharyngeal cancer subject; N: healthy volunteer subject; AUC: The integration area under the ROC curves.

Table S3 Classification results of blood SERS prediction of samples belonging to one pathology type using PCA-LDA method.

Pathology type	Predicted parameters		
	Sensitivity	Specificity	AUC
T1 stage cancer (12 samples vs. 13 samples)	50% (6/12)	30.8% (4/13)	0.558
T2-T4 stage cancer (37 samples vs. 38 samples)	45.9% (17/37)	44.7% (17/38)	0.564
Normal (30 samples vs. 30 samples)	63.3% (19/30)	46.7% (14/30)	0.608

AUC: The integration areas under the ROC curve.

Table S4 Classification results of blood SERS prediction of negative control (rhinitis patients) and previous three pathology groups using PCA-LDA method.

Diagnostic combinations			Predicted parameters		
			Sensitivity	Specificity	AUC
Rhinitis	vs.	Normal	30% (3/10)	55% (33/60)	0.604
Rhinitis	vs.	T1 stage cancer	80% (8/10)	80% (20/25)	0.936
Rhinitis	vs.	T2-T4 stage cancer	90% (9/10)	92% (69/75)	0.976

AUC: The integration areas under the ROC curve.