

Supplementary Materials: Thermal Liquid Biopsy (TLB): A predictive score derived from serum thermograms as a clinical tool for screening lung cancer patients

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Table S1. Main descriptive measures for the 14 TLB-derived parameters.

HC Group	Minimum	Q1	Q2	Average	Q3	Maximum
T _{av}	65.93	67.59	67.95	67.98	68.39	69.08
G ₁	-0.3757	0.1333	0.2588	0.2330	0.3521	0.7714
AUC _{n2}	7.011	19.86	26.89	36.92	43.66	201.7
AP _{n2}	0.2438	0.6233	1.127	3.598	2.762	81.29
AUC _{n3}	14.98	20.39	22.76	24.02	25.94	76.84
AP _{n3}	0.2934	0.5914	0.8038	0.9215	1.016	4.343
AUC _{n4}	2.882	28.69	39.55	43.90	51.97	148.2
AP _{n4}	0.07751	1.457	2.416	3.232	4.028	16.24
AUC _{n5}	22.06	39.20	43.20	49.67	50.93	143.8
AP _{n5}	0.2949	2.265	2.876	4.203	4.148	33.44
DV ₂	0.9857	1.057	1.190	3.244	1.867	71.43
DV ₃	0.9855	1.008	1.043	1.175	1.121	5.101
DV ₄	0.9861	1.043	1.173	1.443	1.375	6.069
DV ₅	0.9825	1.003	1.035	1.377	1.160	10.93

LCP Group	Minimum	Q1	Q2	Average	Q3	Maximum
T _{av}	65.04	67.79	68.16	68.23	68.71	70.63
G ₁	-0.1058	0.2899	0.4436	0.4518	0.5662	3.622
AUC _{n2}	7.011	18.72	24.20	29.82	36.15	98.32
AP _{n2}	0.0952	0.4884	0.9303	1.924	1.902	20.61
AUC _{n3}	8.830	21.59	25.76	34.63	33.09	263.71
AP _{n3}	0.2049	0.7416	0.9723	2.145	1.551	29.33
AUC _{n4}	4.842	25.74	33.30	122.7	46.76	8098.0
AP _{n4}	0.2855	0.9898	1.619	261.2	3.508	28790
AUC _{n5}	18.95	36.73	47.69	101.8	63.12	1858
AP _{n5}	0.1778	2.150	3.120	152.3	6.294	8070
DV ₂	0.9857	1.094	1.204	1.909	1.393	17.32

Dv3	0.9855	1.014	1.072	2.562	1.509	35.50
Dv4	0.9861	1.081	1.184	3.872	1.333	149.7
Dv5	0.9825	1.025	1.197	3.644	1.480	85.04

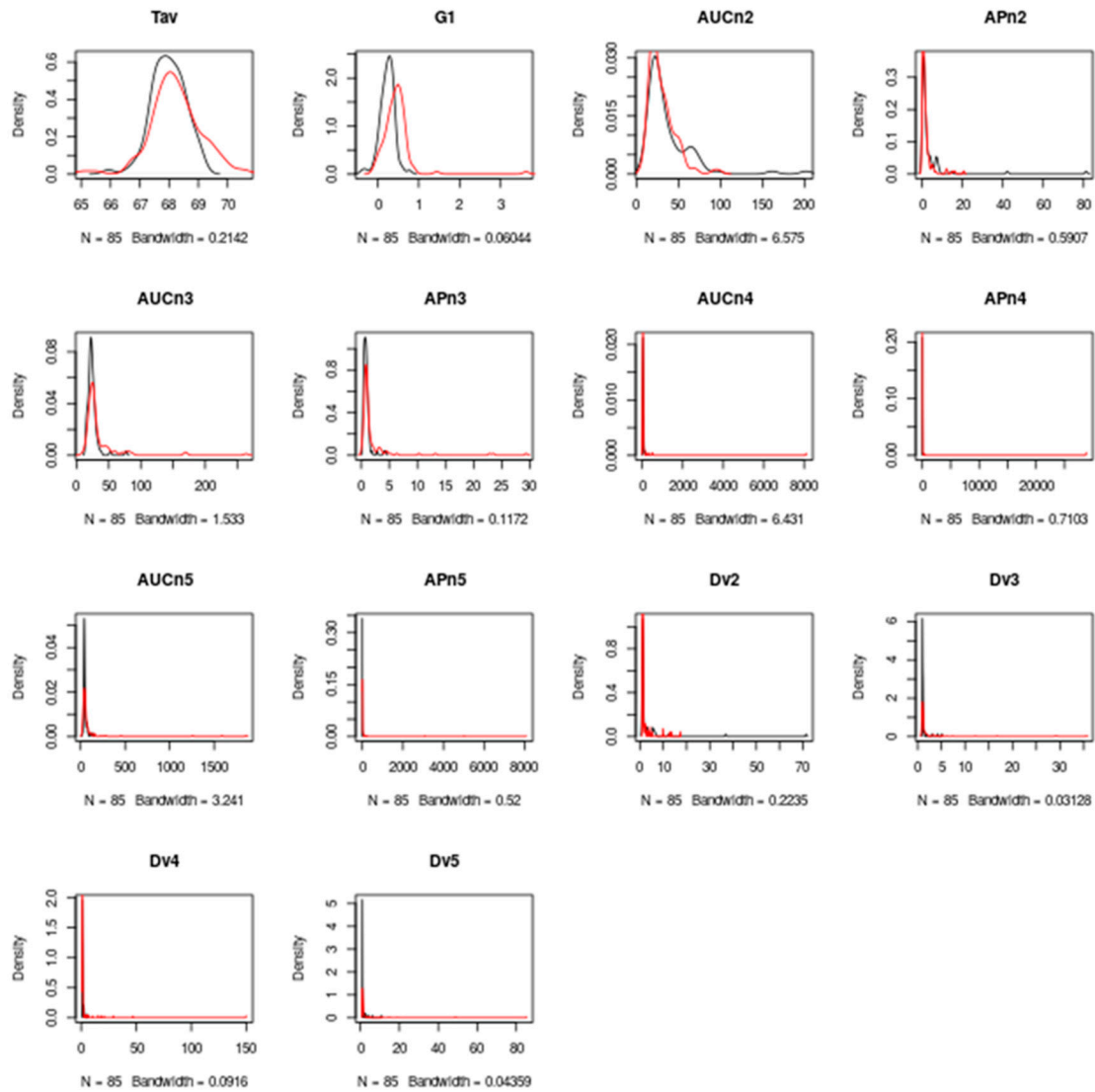


Figure S1. Non-parametric density estimators for the 14 individual TLB-derived parameters. HC group (black) / LCP group (red).

Table S2. Comparative study of the performance of GLM, LDA, SVM, and NBC on the three models.

	Parameter	Success rate	Sensitivity	Specificity
Model 1	GLM	88	89	87
	LDA	84	88	79
	SVM	90	87	95
	NBC	55	24	98
Model 2	Parameter	Success rate	Sensitivity	Specificity

	GLM	69	73	65
	LDA	58	96	6
	SVM	61	97	13
	NBC	55	25	96

	Parameter	Success rate	Sensitivity	Specificity
Model 3	GLM	91	90	92
	LDA	85	88	81
	SVM	90	88	96
	NBC	56	25	96

Four statistical tools (GLM, LDA, SVM, and NBC) were employed for classifying subjects into healthy and diseased individuals using the three models: 1) model 1 with T_{av} , G_1 , AUC_{ni} , and AP_{ni} ; 2) model 2 with Dv_i ; and 3) model 3 with all 14 parameters.

Table S3. PS score vs gender & age (p -value from Kruskal-Wallis test).

Gender	Healthy Controls					Lung Cancer Patients				
	N	Q1	Q2	Q3	p -Value	N	Q1	Q2	Q3	p -Value
Men	45	0.7649	0.8776	0.9380	0.4542	95	0.0075	0.0450	0.1681	0.6620
Women	40	0.6448	0.8722	0.9515		19	0.0101	0.0457	0.2632	

Age	Healthy Controls					Lung Cancer Patients				
	N	Q1	Q2	Q3	p -Value	N	Q1	Q2	Q3	p -Value
< 40	34	0.7022	0.8699	0.9343	0.8498	0				0.2133
40 - 50	17	0.7706	0.8692	0.9062		10	0.0120	0.0443	0.0879	
50 - 60	17	0.6528	0.8707	0.9035		22	0.0090	0.1574	0.4478	
60 - 70	17	0.5411	0.8883	0.9713		54	0.0114	0.0423	0.1564	
70 -	0					28	0.0003	0.0309	0.1375	

Table S4. PS score vs. clinical history information (p -value from Kruskal-Wallis test).

Diagnostic	Lung Cancer Patients				
	N	Q1	Q2	Q3	p -Value
Adenocarcinoma	43	0.0166	0.0672	0.2046	0.2943
Squamous cell carcinoma	32	0.0040	0.0301	0.0899	
Small cell carcinoma	35	0.0078	0.0324	0.1739	
Other non-small cell carcinoma	4	0.0223	0.0823	0.3456	

Stage	Lung Cancer Patients				
	N	Q1	Q2	Q3	p -Value
II	6	0.0008	0.0456	0.0923	0.4278
III	30	0.0096	0.0334	0.1169	
IV	78	0.0079	0.0566	0.1964	

Treatment	Lung Cancer Patients				
	N	Q1	Q2	Q3	p -Value

Adjuvant Chemotherapy	8	0.0018	0.0072	0.0917	0.6424
Neoadjuvant Chemotherapy	3	0.0061	0.0113	0.1764	
Palliative Chemotherapy	77	0.0078	0.0546	0.1845	
Radio- Chemotherapy	26	0.0127	0.0412	0.1327	

Lung Cancer Patients					
Response	N	Q1	Q2	Q3	<i>p</i>-Value
Stable disease	19	0.0004	0.0133	0.0618	0.0967
Death	22	0.0065	0.0648	0.2063	
Disease progression	15	0.0468	0.1419	0.1915	
Complete response	11	0.0038	0.0091	0.0518	
Partial response	46	0.0246	0.0469	0.1981	