

Table S1A: Summary Statistics of predictor variables for the breast Tanner stage groups

		Age		BMI		Breast cancer risk*	
Breast_Stage	sample_size	Mean	SD	Mean	SD	Mean	SD
1	16	11.05	0.64	16.50	1.90	1.70	0.45
2	31	11.19	0.95	17.31	2.25	2.04	0.66
3	31	12.32	1.23	18.90	2.43	1.80	0.51
4	18	13.58	1.38	19.70	1.74	1.88	0.64

		PC1*		PC2*		PC3*	
Breast_Stage	sample_size	Mean	SD	Mean	SD	Mean	SD
1	16	0.19	1.01	0.33	0.43	-0.62	0.69
2	31	0.001	0.649	0.31	0.60	0.11	0.59
3	31	0.10	1.02	-0.23	0.57	0.15	0.65
4	18	-0.37	0.95	-0.41	0.42	0.10	0.80

		PC4*		PC5*		PC6*	
Breast_Stage	sample_size	Mean	SD	Mean	SD	Mean	SD
1	16	0.04	0.68	-0.07	0.92	-0.34	0.88
2	31	-0.04	0.48	-0.08	0.62	-0.27	0.69
3	31	-0.03	0.82	0.01	0.92	0.28	0.82
4	18	0.14	0.86	0.22	0.66	0.24	0.72

		PC7*		PC8*	
Breast_Stage	sample_size	Mean	SD	Mean	SD
1	16	-0.23	0.64	-0.12	0.51
2	31	-0.20	0.78	0.05	1.06
3	31	0.20	0.70	-0.01	0.67
4	18	0.24	0.85	0.25	0.88

*scaled by IQR (Inter-quartile range)

Table S1B: Summary Statistics of predictor variables for the early and late breast stage groups

		Age		BMI		Breast cancer risk*	
Breast_Stage	sample_size	Mean	SD	Mean	SD	Mean	SD
early	47	11.14	0.85	17.04	2.15	1.92	0.61
late	55	12.79	1.41	19.90	3.20	1.83	0.55
		PC1*		PC2*		PC3*	
Breast_Stage	sample_size	Mean	SD	Mean	SD	Mean	SD
early	47	0.07	0.78	0.31	0.54	-0.14	0.71
late	55	0.02	1.00	-0.30	0.50	0.14	0.69
		PC4*		PC5*		PC6*	
Breast_Stage	sample_size	Mean	SD	Mean	SD	Mean	SD
early	47	-0.01	0.55	-0.08	0.73	-0.29	0.75
late	55	0.04	0.79	0.09	0.82	0.21	0.78
		PC7*		PC8*			
Breast_Stage	sample_size	Mean	SD	Mean	SD		
early	47	-0.21	0.73	-0.01	0.91		
late	55	0.20	0.72	0.09	0.73		

*scaled by IQR (Inter-quartile range)

Table S2 A: Correlation Analysis (n=102)

Predictor	Breast Cancer Risk	
	correlation coefficient*	P-value
Age	0.13	0.2001
BMI	-0.03	0.7677
PC1	-0.04	0.7256
PC2	-0.07	0.4779
PC3	0.06	0.5611
PC4	-0.21	0.0328
PC5	0.17	0.0907
PC6	0.04	0.7141
PC7	-0.01	0.8963
PC8	-0.26	0.0082

* Spearman's

Table S2 B: Correlation Analysis in the late subgroup (n=55)

Predictor	Breast Cancer Risk	
	correlation coefficient*	P-value
Age	0.23	0.0849
BMI	0.04	0.7802
PC1	-0.08	0.5450
PC2	-0.06	0.6447
PC3	-0.005	0.9708
PC4	-0.36	0.0074
PC5	0.19	0.1697
PC6	-0.09	0.5014
PC7	0.12	0.4013
PC8	-0.34	0.0114

* Spearman's

Supplementary Table S3A) Correlation R between the PC spectra and chromophore spectra

R	Hb	HbO ₂	Lipid	Water	Collagen
PC1	-0.71	0.07	0.46	-0.22	-0.49
PC2	-0.01	-0.42	-0.06	-0.87	-0.15
PC3	-0.90	0.58	0.63	0.41	-0.58
PC4	-0.24	-0.69	-0.08	0.14	0.44
PC5	-0.32	-0.08	-0.67	0.09	-0.64
PC6	-0.01	0.00	0.34	0.15	-0.05
PC7	0.13	0.04	-0.12	-0.09	-0.28
PC8	0.09	0.02	0.00	0.00	-0.20

Supplementary Table S3B) significance of PC spectra to chromophore spectra correlation as given by the p value

P	Hb	HbO ₂	Lipid	Water	Collagen
PC1	<0.001	0.168	<0.001	<0.001	<0.001
PC2	0.847	<0.001	0.237	<0.001	0.002
PC3	<0.001	<0.001	<0.001	<0.001	<0.001
PC4	<0.001	<0.001	0.084	0.004	<0.001
PC5	<0.001	<0.001	<0.001	0.059	<0.001
PC6	0.813	<0.001	<0.001	0.002	0.293
PC7	0.005	0.422	0.011	0.048	<0.001
PC8	0.059	0.707	0.919	0.945	<0.001