

Breast Cancer Diagnosis by Surface-Enhanced Raman Scattering (SERS) of Urine

Vlad Moisoiu ^{1,2,†}, Andreea Socaciu ^{2,3,†}, Andrei Stefancu ^{1,4}, Stefania D. Iancu ^{1,5}, Imre Boros ^{6,7}, Cristian D. Alecsa ^{6,7}, Claudiu Rachieriu ², Angelica R. Chiorean ⁸, Daniela Eniu ⁹, Nicolae Leopold ^{1,4,*}, Carmen Socaciu ^{10,11,*} and Dan T. Eniu ^{2,12}

¹ Faculty of Physics, Babeș-Bolyai University, 400084 Cluj-Napoca, Romania; vlad.moisoiu@gmail.com (V.M.); stefancu.andrei16@gmail.com (A.S.); stefania.iancu22@yahoo.ro (S.D.I.)

² Faculty of Medicine, Iuliu Hatieganu University of Medicine and Pharmacy, 400349 Cluj-Napoca, Romania; andreeaiso@gmail.com (A.S.); crachieriu@yahoo.com (C.R.); daneniu@gmail.com (D.T.E.)

³ MEDISYN Clinic, 400474 Cluj-Napoca, Romania

⁴ MEDFUTURE Research Center for Advanced Medicine, Iuliu Hatieganu University of Medicine and Pharmacy, 400000 Cluj-Napoca, Romania

⁵ IMOGEN Medical Research Institute, County Clinical Emergency Hospital, 400012 Cluj-Napoca, Romania

⁶ Faculty of Mathematics and Computer Science, Babeș-Bolyai University, 400084 Cluj-Napoca, Romania; imre.boros@math.ubbcluj.ro (I.B.); cristian.alecsa@math.ubbcluj.ro (C.D.A.)

⁷ Tiberiu Popoviciu Institute of Numerical Analysis, 400320 Cluj-Napoca, Romania

⁸ Department of Radiology, Iuliu Hatieganu University of Medicine and Pharmacy, 400349 Cluj-Napoca, Romania; chiorean_angi@yahoo.com

⁹ Department of Biophysics, Iuliu Hatieganu University of Medicine and Pharmacy, 400349 Cluj-Napoca, Romania; daniela.enui@umfcluj.ro

¹⁰ Faculty of Food Science and Technology, University of Agricultural Sciences and Veterinary Medicine, 400372 Cluj-Napoca, Romania

¹¹ BIODIATECH Research Centre for Applied Biotechnology, SC Proplanta, 400478 Cluj-Napoca, Romania

¹² Department of Surgical and Gynecological Oncology, Ion Chiricuta Oncologic Institute, 400015 Cluj-Napoca, Romania

* Correspondence: correspondence: nicolae.leopold@phys.ubbcluj.ro (N.L.); carmen.socaciu@usamvcluj.ro (C.S.); Tel.: +40-264-405300 (N.L.); +40-264-596384 (C.S.)

† these authors contributed equally and are co-first authors.

Table S1. The age and stage of breast cancer patients and controls.

Sample Number	Age of Controls	Age of Breast Cancer Patients	Stage of Breast Cancer
1.	45	33	I A
2.	44	46	II A
3.	50	47	II B
4.	44	60	II A
5.	42	56	III B
6.	48	43	II A
7.	52	51	I A
8.	43	59	III B
9.	42	71	III B
10.	37	80	III A
11.	50	54	III B
12.	44	65	III A
13.	48	67	II B
14.	59	65	III B
15.	48	46	II A
16.	46	58	III A
17.	42	46	I A
18.	45	39	II B
19.	36	73	III A

20.	39	59	II B
21.	48	54	III B
22.	46	64	II B
23.		58	III A
24.		77	II B
25.		63	II B
26.		70	II B
27.		61	II A
28.		50	III A
29.		53	III A
30.		70	III A
31.		44	III B
32.		41	III A
33.		72	III B
34.		56	II B
35.		35	II B
36.		67	II B
37.		40	III B
38.		54	III B
39.		46	III A
40.			III A
41.		66	III B
42.		57	II B
43.		60	III B
44.		53	III B
45.		48	II B
46.		50	III A
47.		65	II A
48.		59	III A
49.		40	III A
50.		38	II A
51.		67	III A
52.		58	II A
53.		46	III A

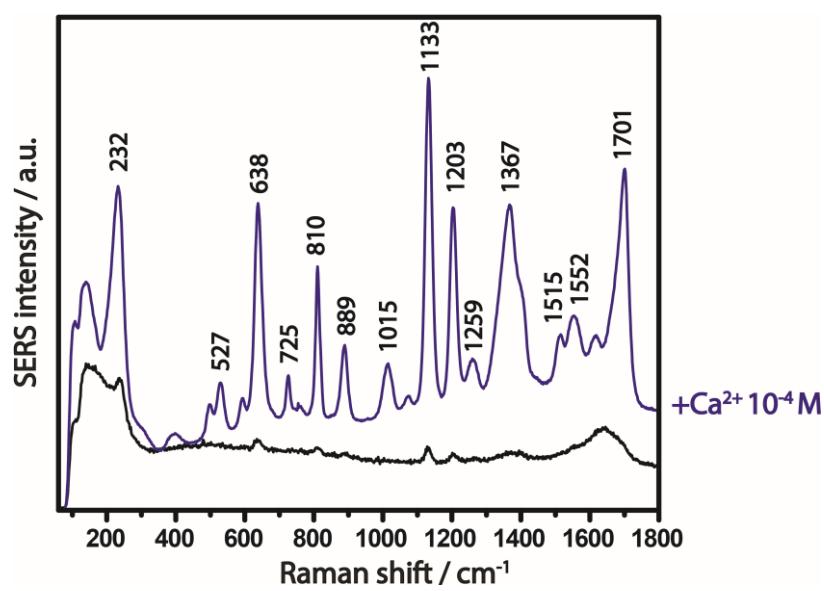


Figure S1. The SERS spectrum of uric acid 10^{-4} M before (black) and after activation with Ca^{2+} 10^{-4} M (blue).

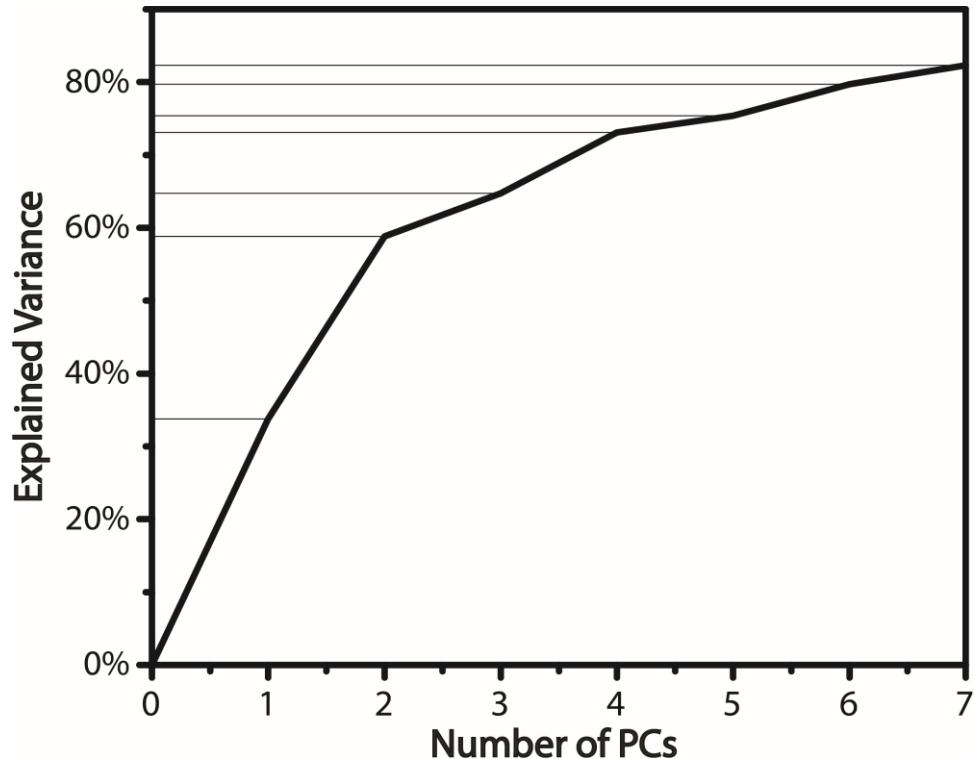


Figure S2. The explained variance by the first 7 principal components (PCs).

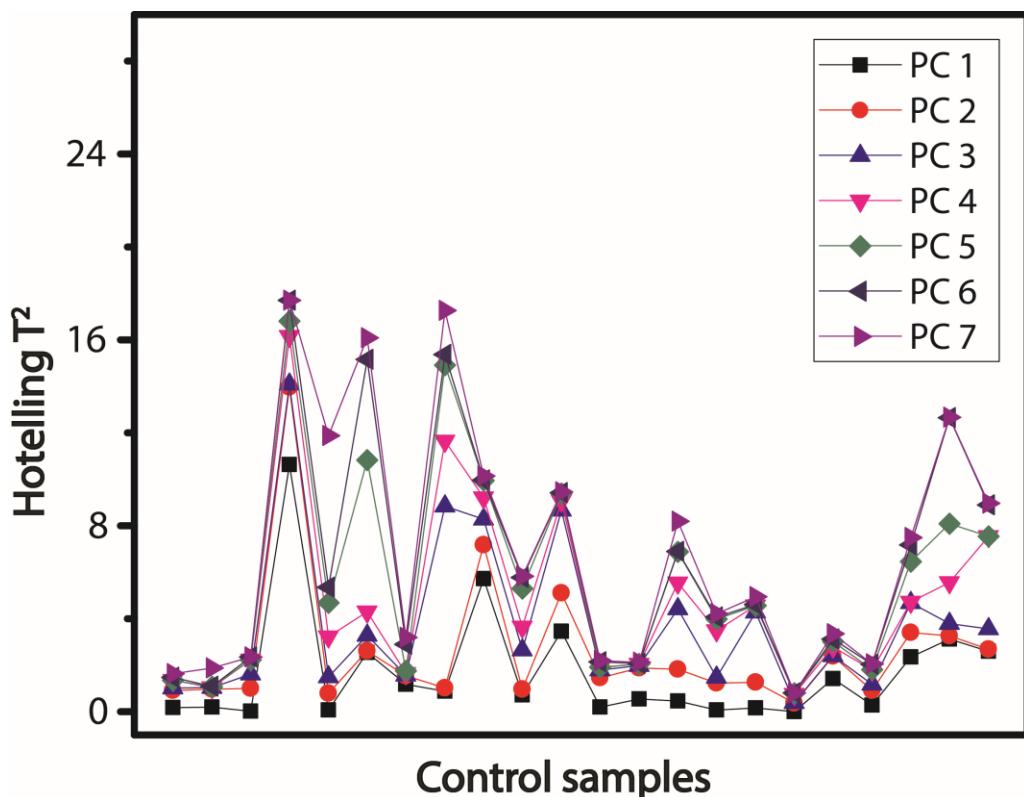


Figure S3. The Hotelling T^2 values of $n = 22$ samples in the control group corresponding to the first 7 principal components (PCs).

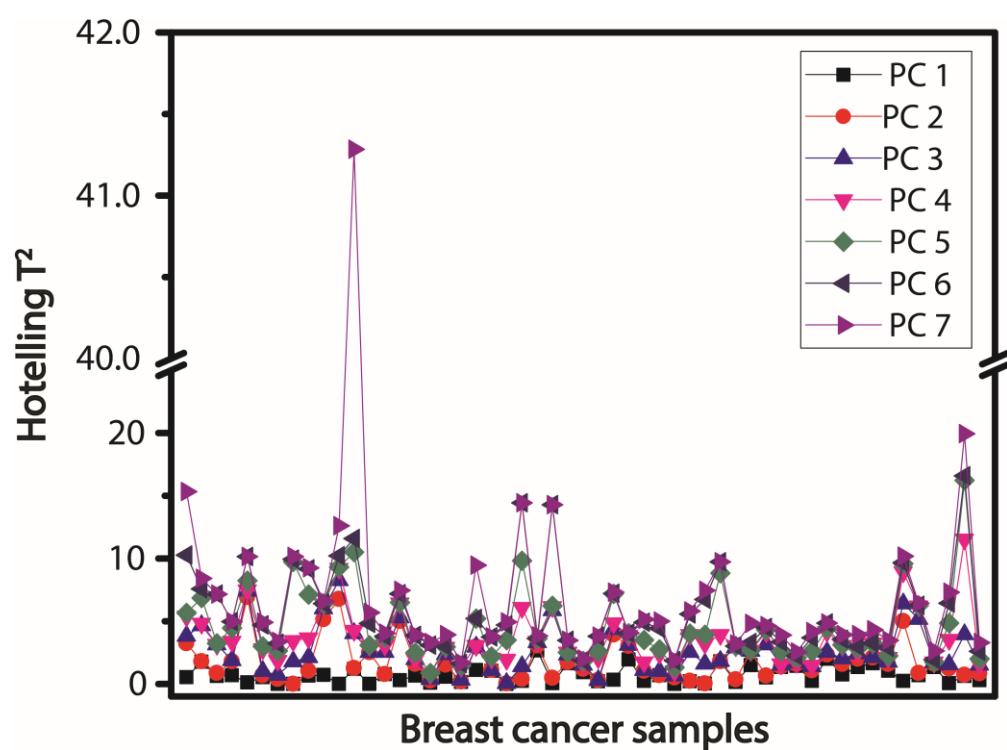


Figure S4. The Hotelling T^2 values of $n = 53$ samples in the breast cancer group corresponding to the first 7 principal components (PCs).