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ELECTRONIC SUPPLEMENTARY INFORMATION

Paper spray mass spectrometry combined with machine learning as a rapid diagnostic for chronic kidney disease

Igor Pereira[1], Jindar N. S. Sboto[1], Jason L. Robinson[2], and Chris G. Gill[1, 3, 4, 5*]

[1] Applied Environmental Research Laboratories (AERL), Chemistry Department, Vancouver Island University, Nanaimo, BC, Canada, V9R 5S5
[2] Health PEI, Charlottetown, PEI, Canada, C1A 7N8
[3] Chemistry Department, University of Victoria, Victoria, BC, Canada, V8P 5C2
[4] Chemistry Department, Simon Fraser University, Burnaby, BC, Canada, V5A 1S6
[5] Department of Occupational and Environmental Health Sciences, University of Washington, Seattle, WA, United States, 98195-1618

***Address correspondence to:**

Professor Chris G. Gill, Ph.D., P. Chem.
Co-Director, Applied Environmental Research Laboratories (AERL)
Department of Chemistry
Vancouver Island University
900 Fifth Street, Nanaimo, BC, Canada, V9R 5S5

Ph: 250-753-3245
chris.gill@viu.ca

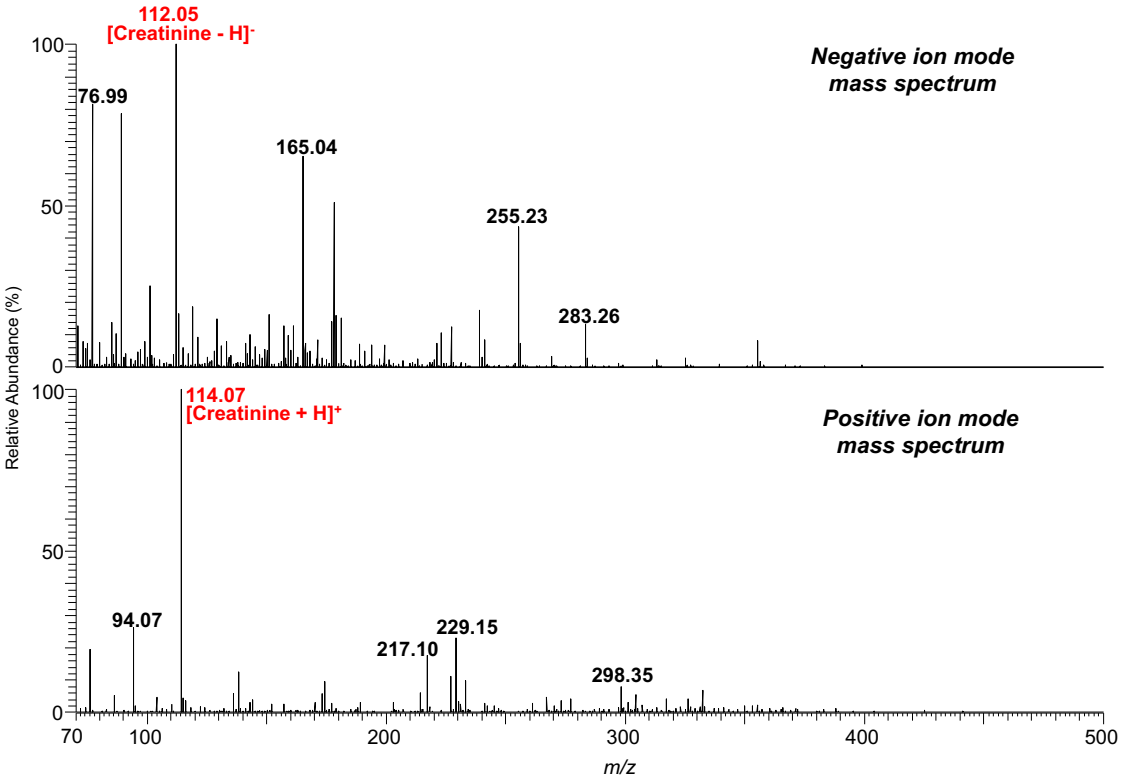

Fig. S1 Representative negative and positive ion mode PS-MS mass spectra for obtained for a healthy anonymous patient urine sample.

Table S1 Albumin-to-creatinine ratio (ACR) concentrations (mg $mmol^{-1}$) in 80 (healthy = 40; diseased = 40) anonymous human patient urine samples

Sample	ACR values (mg $mmol^{-1}$)	Classification
1	0.4	Healthy
2	0.5	Healthy
3	0.5	Healthy
4	0.5	Healthy
5	0.5	Healthy
6	0.5	Healthy
7	0.5	Healthy
8	0.6	Healthy
9	0.6	Healthy
10	0.7	Healthy
11	0.7	Healthy
12	0.7	Healthy
13	0.7	Healthy
14	0.8	Healthy
15	0.8	Healthy
16	0.8	Healthy
17	0.8	Healthy
18	0.8	Healthy
19	0.8	Healthy
20	0.9	Healthy
21	0.9	Healthy
22	1.0	Healthy
23	1.0	Healthy
24	1.0	Healthy
25	1.0	Healthy
26	1.0	Healthy
27	1.0	Healthy
28	1.1	Healthy
29	1.1	Healthy
30	1.1	Healthy
31	1.2	Healthy
32	1.2	Healthy
33	1.2	Healthy
34	1.2	Healthy
35	1.3	Healthy
36	1.5	Healthy
37	1.5	Healthy
38	1.6	Healthy
39	1.6	Healthy
40	1.8	Healthy

41	3.7	Diseased
42	4.0	Diseased
43	5.9	Diseased
44	7.5	Diseased
45	7.9	Diseased
46	10.3	Diseased
47	12.4	Diseased
48	13.8	Diseased
49	15.4	Diseased
50	15.6	Diseased
51	17.6	Diseased
52	23.9	Diseased
53	24.0	Diseased
54	24.8	Diseased
55	25.7	Diseased
56	27.4	Diseased
57	30.3	Diseased
58	30.4	Diseased
59	31.6	Diseased
60	32.0	Diseased
61	34.1	Diseased
62	34.7	Diseased
63	42.4	Diseased
64	56.2	Diseased
65	66.4	Diseased
66	69.0	Diseased
67	76.1	Diseased
68	80.2	Diseased
69	98.8	Diseased
70	108.0	Diseased
71	126.5	Diseased
72	153.3	Diseased
73	172.0	Diseased
74	206.9	Diseased
75	224.0	Diseased
76	260.5	Diseased
77	270.1	Diseased
78	319.4	Diseased
79	375.0	Diseased
80	1342.3	Diseased

Table S2 Albumin-to-creatinine ratio (ACR) concentrations (mg $mmol^{-1}$) in 24 (healthy = 12; diseased = 12) anonymous human patient urine samples used as test dataset

Sample	ACR values (mg $mmol^{-1}$)	Classification
1	0.5	Healthy
2	0.8	Healthy
3	0.9	Healthy
4	0.9*	Healthy
5	0.9*	Healthy
6	1.0	Healthy
7	1.1	Healthy
8	1.2*	Healthy
9	1.3*	Healthy
10	1.5	Healthy
11	1.8*	Healthy
12	1.9*	Healthy
13	3.2*	Diseased
14	3.3*	Diseased
15	3.7*	Diseased
16	4.2*	Diseased
17	4.6*	Diseased
18	7.9	Diseased
19	12.4	Diseased
20	13.8	Diseased
21	18.7*	Diseased
22	32.0	Diseased
23	80.2	Diseased
24	98.8	Diseased

*Samples from a new batch. The remaining samples are from the batch shown in Table S1.

Table S3 Tentative annotation for 10 features (*m/z*) measured in negative ionization mode PS-MS selected by the random forest machine learning method

Tentative attribution	Molecular formula	*m/z* $[M-H]^-$	Mass error (ppm)	MDA*	Level	References**
Azelaic acid	$C_9H_{16}O_4$	187.09769	0.576	0.0022960	Down in diseased	S1
3-Hydroxycapric acid	$C_{10}H_{20}O_3$	187.13409	0.653	0.0021812	Up in diseased	S2
1,4-Dichlorobenzene	$C_6H_4Cl_2$	144.96185	0.835	0.0020376	Up in diseased	S3
cis-2-Methylaconitic acid	$C_7H_8O_6$	187.02491	0.528	0.0019953	Down in diseased	S4
Dimethyl sulfone	$C_2H_6O_2S$	93.00162	0.501	0.0019354	Up in diseased	S5
2,4-Dichlorophenol	$C_6H_4Cl_2O$	160.95671	0.413	0.0018158	Up in diseased	S2
3-Hydroxyisovaleric acid	$C_5H_{10}O_3$	117.05580	0.705	0.0016848	Down in diseased	S6
L-1-pyrroline-5-carboxylate	$C_5H_7NO_2$	112.04047	0.609	0.0016550	Down in diseased	S7
p-Aminobenzoic acid	$C_7H_7NO_2$	136.04051	0.795	0.0012424	Down in diseased	S8
4-Hydroxyphenylpyruvic acid	$C_9H_8O_4$	179.03509	0.603	0.0010013	Down in diseased	S9

*Mean Decrease Accuracy (random forest ranking score)
**Published data relating each annotated compound to kidney disease

Table S4 Albumin-to-creatinine ratio (ACR) concentrations (mg $mmol^{-1}$) in anonymous human patient urine samples (*N* = 60) subdivided into normoalbuminuria (<3 mg $mmol^{-1}$, *N* = 20), microalbuminuria (3-30 mg $mmol^{-1}$, *N* = 20), and macroalbuminuria (>30 mg $mmol^{-1}$, *N* = 20)

Sample	ACR values (mg $mmol^{-1}$)	Classification
1	0.4	Normoalbuminuria
2	0.5	Normoalbuminuria
3	0.5	Normoalbuminuria
4	0.5	Normoalbuminuria
5	0.5	Normoalbuminuria
6	0.5	Normoalbuminuria
7	0.5	Normoalbuminuria
8	0.6	Normoalbuminuria
9	0.6	Normoalbuminuria
10	0.7	Normoalbuminuria
11	0.7	Normoalbuminuria
12	0.7	Normoalbuminuria
13	0.7	Normoalbuminuria
14	0.8	Normoalbuminuria
15	0.8	Normoalbuminuria
16	0.8	Normoalbuminuria
17	0.9	Normoalbuminuria
18	1.5	Normoalbuminuria
19	1.6	Normoalbuminuria
20	1.6	Normoalbuminuria
21	3.3	Microalbuminuria
22	3.7	Microalbuminuria
23	4.0	Microalbuminuria
24	4.2	Microalbuminuria
25	4.6	Microalbuminuria
26	5.9	Microalbuminuria
27	6.9	Microalbuminuria
28	7.5	Microalbuminuria
29	7.9	Microalbuminuria
30	10.3	Microalbuminuria
31	12.4	Microalbuminuria
32	13.8	Microalbuminuria
33	15.4	Microalbuminuria
34	15.6	Microalbuminuria
35	17.6	Microalbuminuria
36	23.9	Microalbuminuria
37	24.0	Microalbuminuria
38	24.8	Microalbuminuria

39	25.7	Microalbuminuria
40	27.4	Microalbuminuria
41	34.1	Macroalbuminuria
42	34.7	Macroalbuminuria
43	42.4	Macroalbuminuria
44	56.2	Macroalbuminuria
45	66.4	Macroalbuminuria
46	69.0	Macroalbuminuria
47	76.1	Macroalbuminuria
48	80.2	Macroalbuminuria
49	98.8	Macroalbuminuria
50	108.0	Macroalbuminuria
51	126.5	Macroalbuminuria
52	153.3	Macroalbuminuria
53	172.0	Macroalbuminuria
54	206.9	Macroalbuminuria
55	224.0	Macroalbuminuria
56	260.5	Macroalbuminuria
57	270.1	Macroalbuminuria
58	319.4	Macroalbuminuria
59	375.0	Macroalbuminuria
60	1342.3	Macroalbuminuria

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