Electronic Supporting Information

for

Polydopamine Assisted Functionalization of Boronic Acid on Magnetic Nanoparticles for the Selective Extraction of Ribosylated Metabolites from Urine

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Fig. S1 FTIR spectra of materials (A) Fe_3O_4 and (B) Fe_3O_4@PDA-FPBA nanoparticles

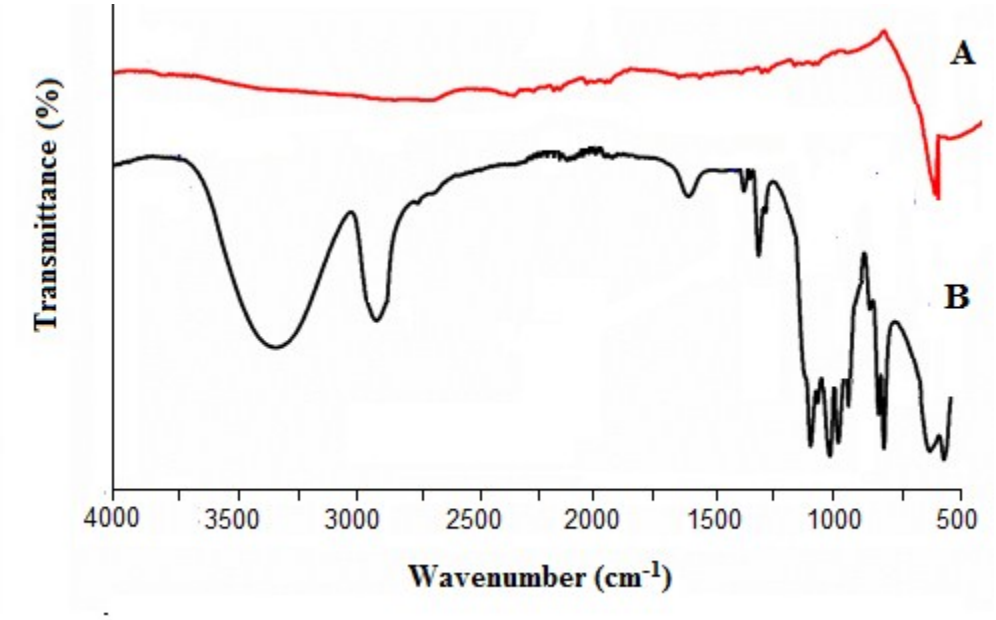

Fig. S2 LC-UV chromatogram of standard nucleosides to assess the retention times prior to enrichment process

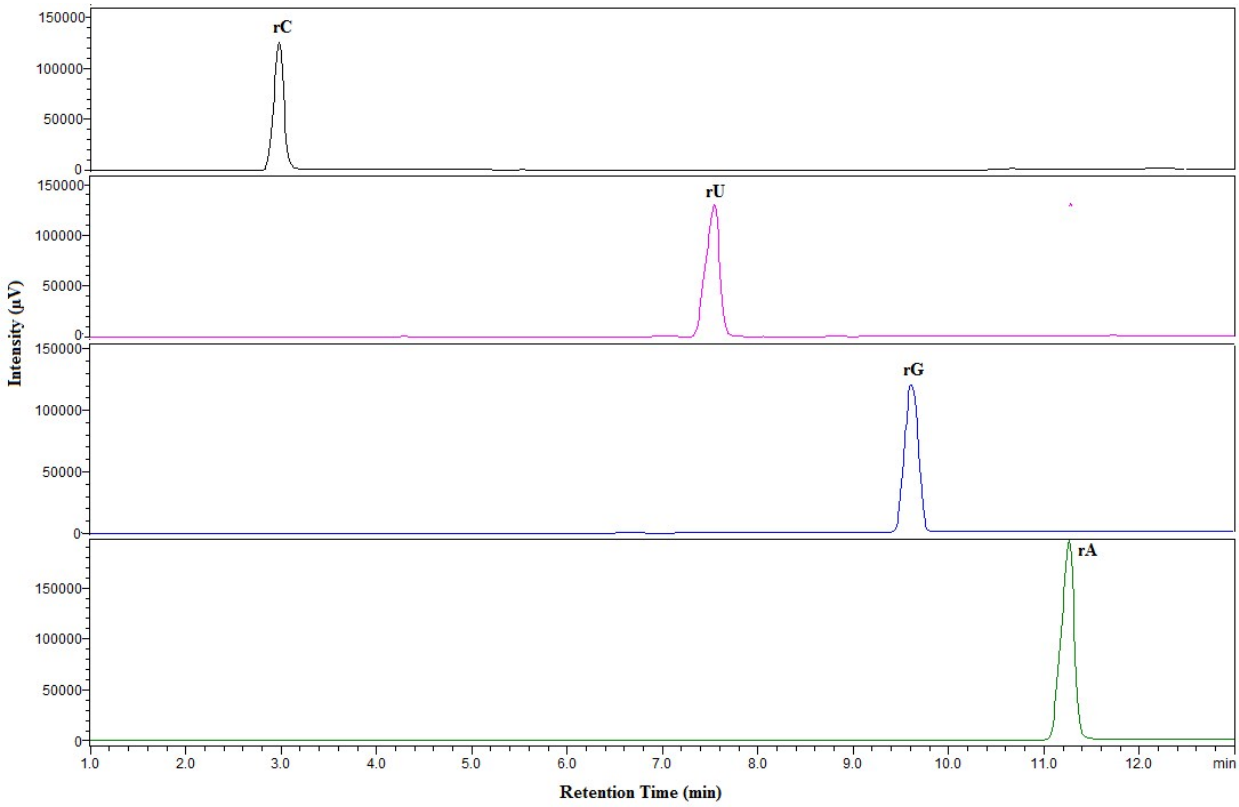

Fig. S3 Extracted ion chromatogram of identified nucleosides from human urine

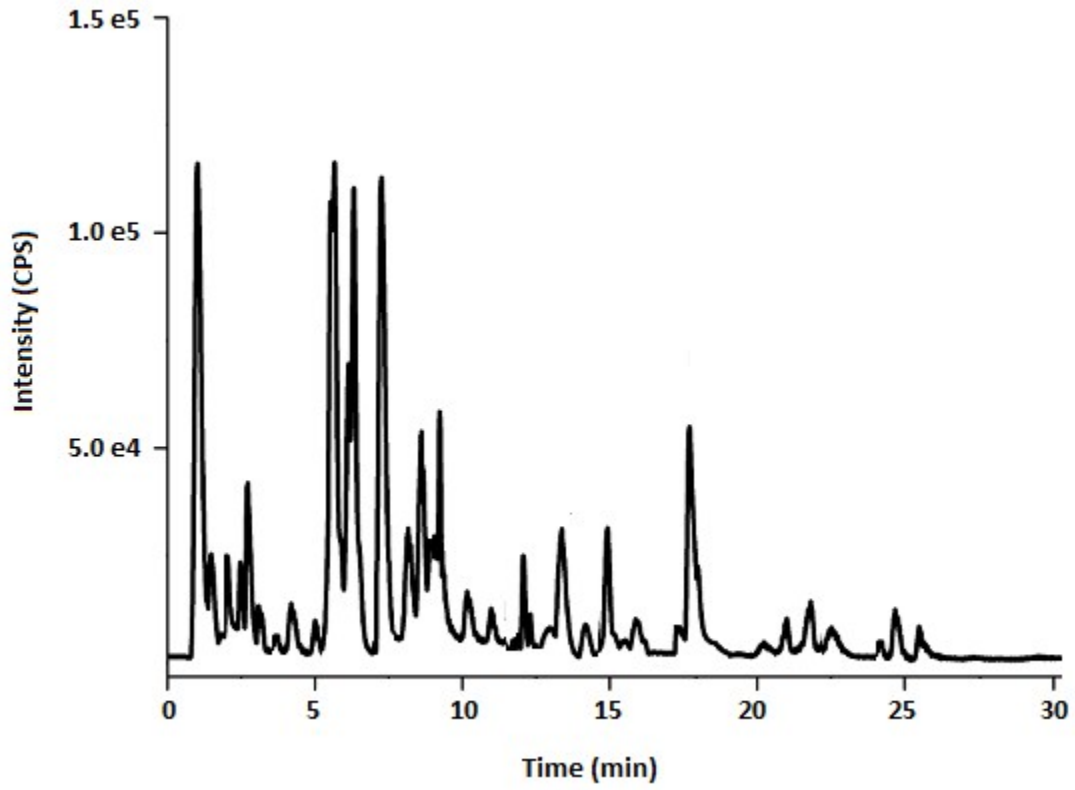

Table S1 Detail of age and gender of lung cancer patients and healthy controls

No	Gender	Age
Lung Cancer		
1	Female	53
2	Female	66
3	Female	51
4	Male	38
5	Male	54
6	Male	53
7	Male	62
8	Male	59
9	Male	52
10	Male	50

Healthy Controls		
1	Female	53
2	Female	66
3	Female	51
4	Female	38
5	Female	54
6	Female	53
7	Male	62
8	Male	59
9	Male	52
10	Male	50

Table S2 MRM parameters for the analysis of standard nucleosides

Compounds	Precursor ion	Product ion	DP (V)	EP (V)	CE (V)	CXP (V)
Adenosine (A)	268.0	136.0	24	6	24	5
Cytidine (C)	244.2	112.2	24	6	22	5
Guanosine (G)	284.2	152.2	28	6	20	5
Uridine (U)	245.2	113.2	30	5	20	4
1-Methyladenosine (m1A)	282.1	152.0	25	10	25	3
5-Methyluridine (m5U)	259.2	127.2	20	6	20	4

Table S3 Comparison of adsorption capacity of Fe_3O_4@PDA-FPBA with previously reported materials

No.	Material	Nucleoside	Adsorption Capacity (μg/g)	Reference
1	Borated Titania	Adenosine	2000	[1]
2	Boronic Acid Avidity on Dendrimer Nanoparticles	Adenosine	1.75	[2]
3	Titania SPE Column	Adenosine	6000	[3]
4	Fe_3O_4@SiO_2@PEI-FPBA	Adenosine	1340	[4]
5	Boronic Acid Functionalized Magnetic Attapulgite	Adenosine	13780	[5]
6	Hybrid TiO_2–ZrO_2 Nanoparticles	Adenosine	35	[6]
7	BA Functionalized Magnesia-Zirconia Composite	Adenosine Cytidine Guanidine Uridine	123.5 114.8 103.5 107.8	[7]
8	Fe_3O_4 microspheres	Adenosine Cytidine Guanidine Uridine	43.9 48.9 41.1 43.4	[8]
9	Zr-Fe_3O_4 microspheres	Adenosine Cytidine Guanidine Uridine	142.1 156.2 159.4 108.5	[8]
10	Fe_3O_4@PDA-FPBA	Adenosine Cytidine Guanidine Uridine	197.3 183.9 163.1 186.5	This study

Table S4 Ion-pairs with neutral loss detected by LC-MS/MS after extraction with Fe_3O_4 @PDA-FPBA nanoparticles

No.	Retention Time (min)	Precursor ions	Product ions
1	2.9	244.1115	112.1203
2	2.4	255.1029	123.0665
3	2.3	288.1985	156.0097
4	2.5	288.9656	157.0401
5	2.7	301.0751	169.0332
6	3.5	274.1034	142.0633
7	4.5	257.9985	126.0670
8	4.7	286.1385	154.0980
9	5.6	345.9935	214.0861
10	5.0	261.0512	129.0134
11	6.3	302.5920	170.0829
12	6.9	284.1020	152.0812
13	7.9	247.0909	115.1501
14	8.5	326.0937	194.0287
15	14.8	298.0952	136.0603
16	16.1	384.1142	252.1081
17	17.9	282.3101	150.1009
18	10.0	269.0881	137.2984
19	10.9	271.1009	139.1569
20	12.6	272.0842	140.0419
21	12.9	296.1331	164.0911
22	17.6	288.3212	126.6546
23	11.7	271.1032	139.0527
24	13.5	285.1025	153.1190
25	14.0	251.9986	136.1228
26	14.4	286.1034	154.0771
27	14.3	285.1177	153.0760
28	15.9	300.1007	168.1294
29	14.3	313.1302	151.0722
30	14.4	269.0873	137.0450

31	18.1	258.1310	126.0417
32	15.6	247.0901	115.0487
33	14.3	317.1012	185.0753
34	15.0	304.1801	172.0319
35	20.5	426.1756	294.1331, 193.0837,150.0752
36	20.8	298.1175	166.0743, 148.0633
37	21.7	299.8727	168.0931
38	23.3	257.1163	125.0690
39	23.5	336.1636	204.1260
40	23.5	326.1455	194.0995
41	24.3	300.0992	168.1360
42	25.5	314.1532	182.1290
43	15.2	328.1092	196.0666
44	15.5	318.1039	172.0792
45	16.6	328.0099	196.2276
46	16.6	326.1480	194.1060, 166.0744
47	16.6	333.0921	201.0496
48	17.1	272.1222	140.0834
49	17.2	413.1721	281.1013
50	17.7	301.0799	169.0369
51	18.0	314.1120	182.0700
52	19.2	312.1103	164.0913, 150.0792
53	20.0	358.1430	226.1031
54	25.8	337.2192	175.1176
55	23.3	257.1163	125.0690
56	16.6	333.0921	201.0496
57	25.6	337.1390	175.0853
58	17.6	301.0799	169.0369
59	16.6	333.0921	201.0496
60	15.2	328.1092	196.0666
61	14.3	285.1177	153.0760
62	11.5	271.1009	139.0596
63	4.6	346.1235	214.0861
64	16.6	326.1480	194.1060

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