Combination of Supporting Vector Regression (SVR) and Microwave Plasma Atomic Emission Spectrometry (MWP-AES) for the Quantitative Elemental Analysis in Solid Samples Using Continuous Direct Solid Sampling (CDSS) Technique

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Table of content

1.

Table S1 Elemental information of the testing samples

No.	Sample 1	Sample 2	Ratio	Pb（μg/g）	Cu（μg/g）	Cr（μg/g）	C_{org} (%)	As（μg/g）	Cd（μg/g）	Zn（μg/g）
1	GSS-14	GSS-7	1:1	22.50	62.20	240.00	0.72	5.65	0.14	119.00
2	GSS-14	GSS-7	1:2	19.67	73.80	296.67	0.69	5.37	0.11	126.67
3	GSS-14	GSS-7	1:3	18.25	79.60	325.00	0.68	5.23	0.10	130.50
4	GSS-14	GSS-7	1:4	17.40	83.08	342.00	0.67	5.14	0.10	132.80
5	GSS-14	GSS-7	1:5	16.83	85.40	353.33	0.67	5.08	0.09	134.33
6	GSS-14	GSS-7	1:6	16.43	87.06	361.43	0.66	5.04	0.09	135.43
7	GSS-14	GSS-7	2:1	25.33	50.60	183.33	0.74	5.93	0.16	111.33
8	GSS-14	GSS-7	3:1	26.75	44.80	155.00	0.75	6.08	0.17	107.50
9	GSS-14	GSS-7	4:1	27.60	41.32	138.00	0.76	6.16	0.17	105.20
10	GSS-14	GSS-7	5:1	28.17	39.00	126.67	0.77	6.22	0.18	103.67
11	GSS-14	GSS-7	6:1	28.57	37.34	118.57	0.77	6.26	0.18	102.57
12	GSS-2	GSS-6	1:1	167.00	203.15	61.00	0.65	116.85	0.11	69.50
13	GSS-2	GSS-6	1:2	216.00	265.43	65.67	0.70	151.23	0.11	78.67
14	GSS-2	GSS-6	1:3	240.50	296.58	68.00	0.73	168.43	0.12	83.25
15	GSS-2	GSS-6	1:4	255.20	315.26	69.40	0.75	178.74	0.12	86.00
16	GSS-2	GSS-6	1:5	265.00	327.72	70.33	0.76	185.62	0.12	87.83
17	GSS-2	GSS-6	1:6	272.00	336.61	71.00	0.76	190.53	0.12	89.14
18	GSS-2	GSS-6	2:1	118.00	140.87	56.33	0.60	82.47	0.10	60.33
19	GSS-2	GSS-6	3:1	93.50	109.73	54.00	0.57	65.28	0.09	55.75
20	GSS-2	GSS-6	4:1	78.80	91.04	52.60	0.55	54.96	0.09	53.00
21	GSS-2	GSS-6	5:1	69.00	78.58	51.67	0.54	48.08	0.09	51.17
22	GSS-2	GSS-6	6:1	62.00	69.69	51.00	0.54	43.17	0.09	49.86
23	GSS-3	GSS-8	1:1	23.50	17.85	50.00	0.41	2.23	0.10	49.50
24	GSS-3	GSS-8	1:2	22.67	20.00	56.00	0.37	1.51	0.11	55.67
25	GSS-3	GSS-8	1:3	22.25[a]	21.08	59.00	0.35	1.15	0.11	58.75
26	GSS-3	GSS-8	1:4	22.00	21.72[a]	60.80	0.34	0.93	0.12	60.60
27	GSS-3	GSS-8	1:5	21.83	22.15	62.00	0.34	0.78	0.12	61.83
28	GSS-3	GSS-8	1:6	21.71	22.46	62.86	0.33	0.68	0.12	62.71
29	GSS-3	GSS-8	2:1	24.33	15.70	44.00	0.44	2.95	0.08	43.33
30	GSS-3	GSS-8	3:1	24.75	14.63	41.00	0.46	3.32	0.08	40.25
31	GSS-3	GSS-8	4:1	25.00	13.98	39.20	0.47	3.53	0.07	38.40
32	GSS-3	GSS-8	5:1	25.17[a]	13.55	38.00	0.48[a]	3.68	0.07	37.17
33	GSS-3	GSS-8	6:1	25.29	13.24	37.14	0.48	3.78	0.07	36.29
34	Mudstone	GSS-6	1:1	157.00	212.40	67.45	0.41	110.00	0.11	48.50
35	Mudstone	GSS-6	2:1	104.67	153.20	64.93	0.27	73.33	0.10	32.33
36	Mudstone	GSS-6	3:1	78.50	123.60	63.68	0.20	55.00	0.10	24.25
37	Mudstone	GSS-6	4:1	62.80	105.84	62.92[a]	0.16	44.00	0.10	19.40
38	Mudstone	GSS-6	5:1	52.33	94.00	62.42	0.14	36.67	0.10	16.17
39	Mudstone	GSS-6	6:1	44.86	85.54	62.06	0.12	31.43	0.10	13.86
40	Mudstone	GSS-6	7:1	39.25	79.20	61.79	0.10	27.50	0.10	12.13
41	Mudstone	GSS-6	8:1	34.89	74.27	61.58	0.09	24.44	0.09	10.78
42	Mudstone	GSS-6	9:1	31.40	70.32	61.41[a]	0.08	22.00	0.09	9.70
43	Mudstone	GSS-6	10:1	28.55	67.09	61.27	0.07	20.00	0.09	8.82

[a] Samples with elemental contents marked with [a] were selected as validation dataset.

2.

Table S2 Instrumental parameters investigated in this experiment

Instrumental parameters	Applied range
Microwave Frequency (MHz)	2450
Microwave Power (W)	53~120
Argon Flow Rate (mL/min)	150~350
Inner Diameter of Discharge Tube (mm)	1
Spectral Range	175~605 nm
Entrance Slit Width	10 μm
CCD Integration Time	50 ms
CCD Average	1

3.

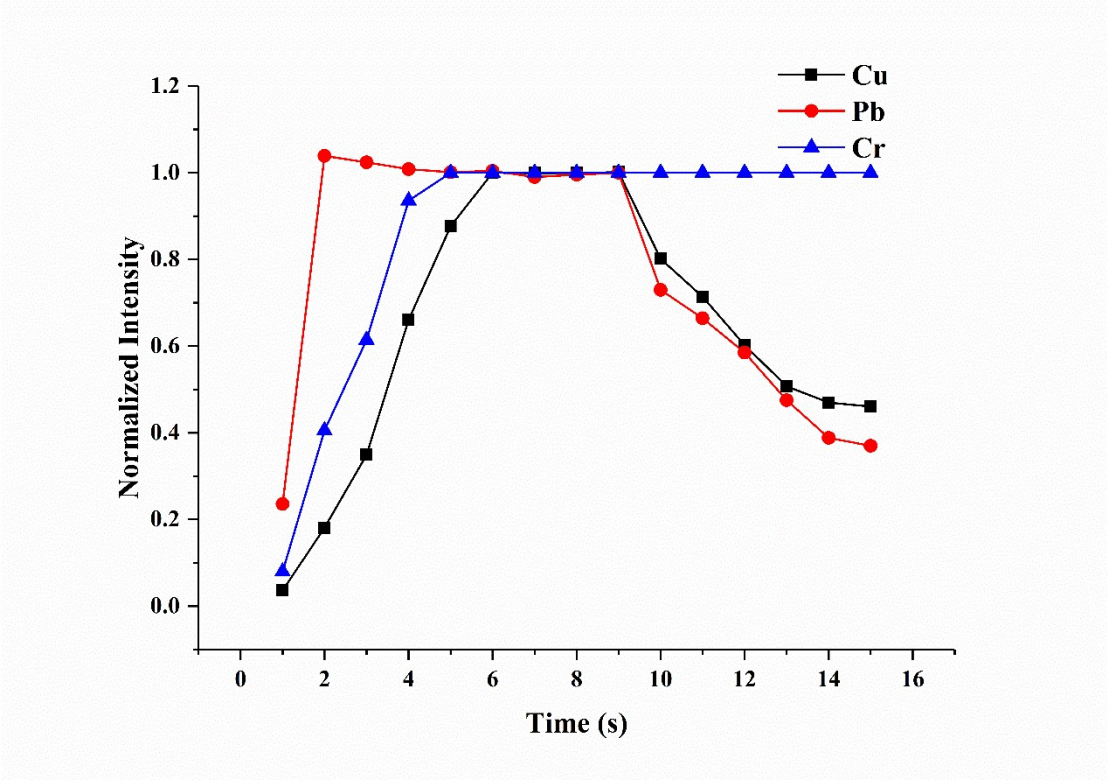

Fig. S1 Selection of the optimal spectral collecting time (Ar flow rate: 200 mL/min, microwave output power: 120 W)

4.

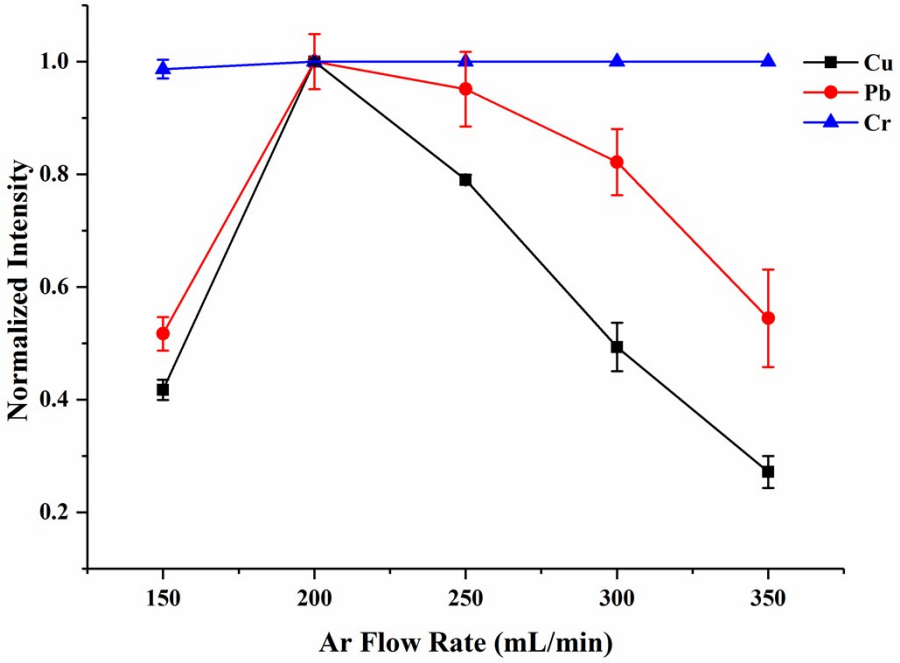

Fig. S2 Influence of Ar flow rate on the normalized intensity of Cu, Pb and Cr (Sample: GSS-5, microwave output power: 120 W)

5.

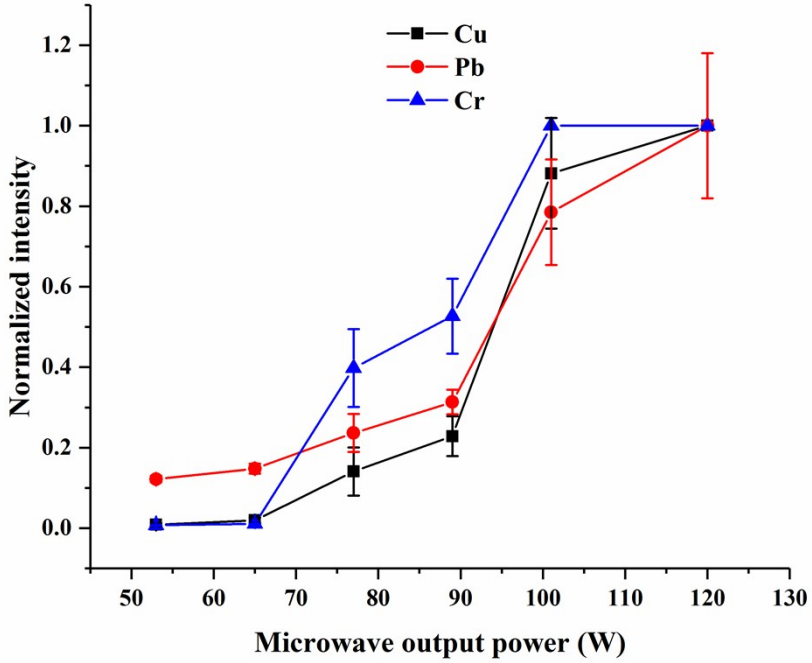

Fig. S3 Influence of microwave output power on the normalized intensity of Cu, Pb and Cr (Sample: GSS-5, Ar flow rate: 200 mL/min)

6.

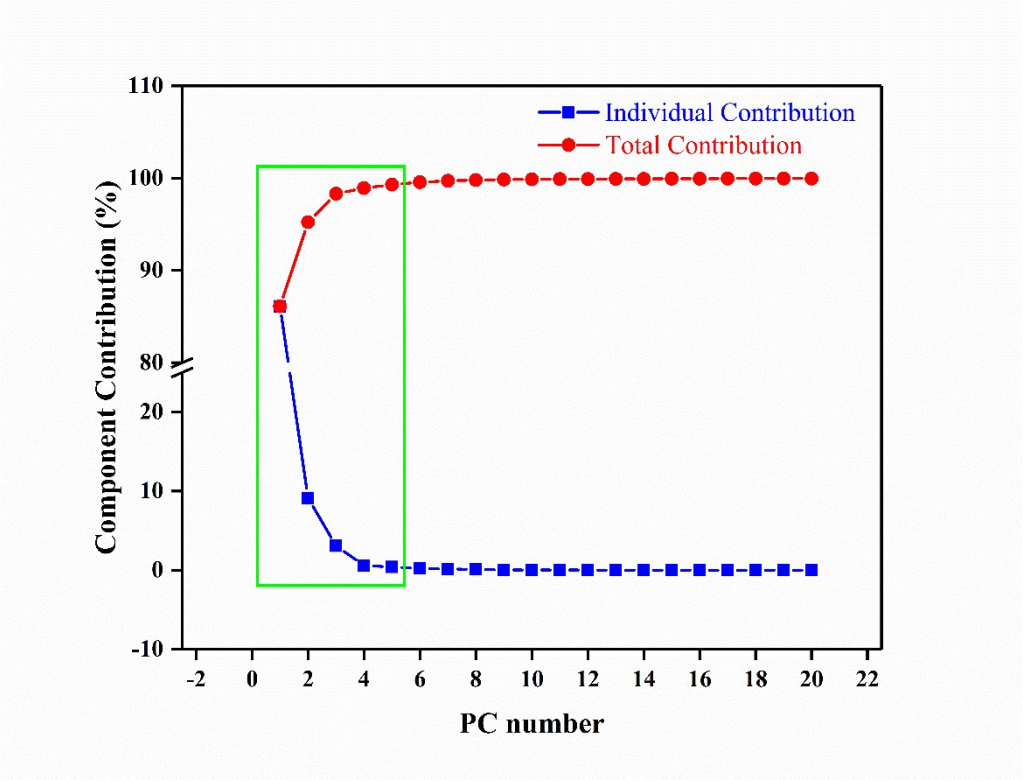

Fig. S4 PCA analysis result

7.

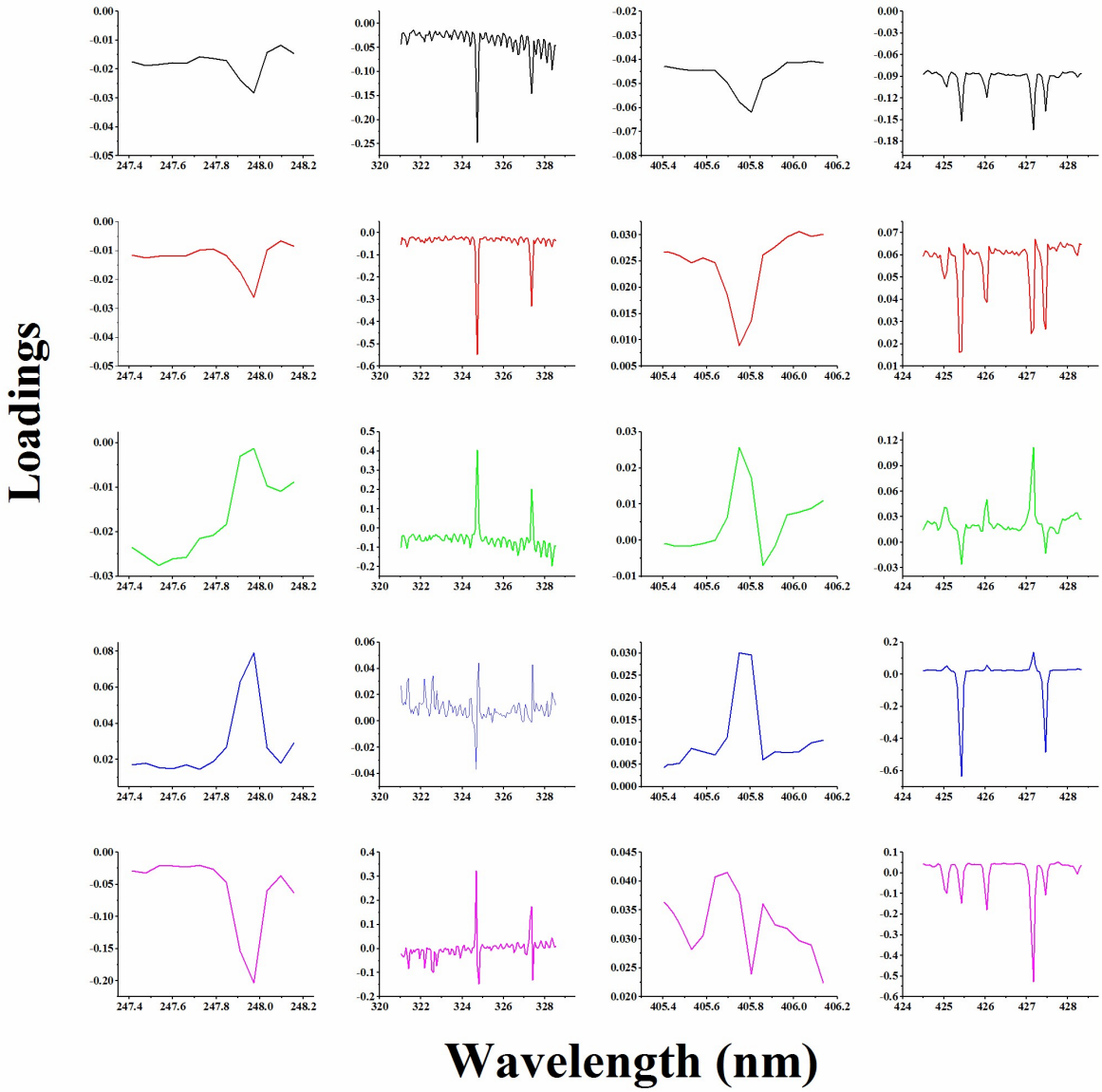

Fig. S5 Spectral loadings for the first five PCs