

Table S1 Major and trace constituents of all kidney stones and the details of corresponding patient's (gender and age).

No	Gender	Age	Ca %	Mg µg/g	Na µg/g	K µg/g	Fe µg/g	Cu µg/g	Zn µg/g	Ba µg/g	Ti ng/g	Cr ng/g	Mo ng/g	Cd ng/g	Pb µg/g
1	Male	61	0.3	481.2	813.2	351.7	3.3	5.75	2.3	0.04	0.0	0.0	143.5	9.5	0.00
2	Male	70	25.8	345.0	990.4	167.2	10.8	0.35	29.7	1.71	0.0	0.0	195.5	262.8	0.65
3	Female	34	25.6	363.1	1436.1	64.0	4.5	0.45	25.8	0.51	184.6	0.0	269.5	154.8	0.68
4	Male	41	25.1	336.2	1078.8	224.6	8.9	0.81	38.2	0.34	68.4	66.7	248.9	142.5	1.05
5	Male	67	28.3	1788.7	3819.3	295.6	20.2	0.45	873.1	15.35	723.4	317.6	1264.5	413.8	10.16
6	Female	27	28.1	4469.2	4765.7	830.2	12.6	0.32	771.3	3.70	845.1	0.0	597.7	490.9	13.53
7	Female	64	26.3	258.9	862.1	222.1	4.4	0.39	23.3	0.12	17.5	0.0	371.3	137.4	1.05
8	Female	60	25.0	355.2	1440.4	199.8	7.9	0.68	23.4	0.31	38.9	34.6	419.2	176.8	3.43
9	Male	68	27.3	1209.1	2544.6	180.9	17.3	0.41	222.2	1.32	358.3	0.0	373.8	405.0	8.33
10	Female	51	30.5	1856.6	5048.3	397.6	36.0	0.35	1009.0	3.06	275.7	0.0	797.8	268.4	10.31
11	Male	57	28.1	3403.2	5664.9	221.1	30.9	1.00	1150.9	4.79	831.7	215.1	613.8	937.2	15.59
12	Male	39	8.4	53.1	655.8	202.2	6.0	2.29	8.0	0.12	0.0	0.0	170.8	92.7	0.06
13	Male	64	25.8	450.4	1290.3	403.1	8.0	0.36	25.2	0.79	0.0	0.0	193.1	460.3	1.18
14	Male	59	7.5	48.4	1205.5	281.6	16.3	2.25	5.2	0.06	0.0	1043.4	297.6	40.3	0.22
15	Male	64	25.2	48.2	1655.4	768.6	79.3	0.53	22.4	0.25	55.0	0.0	300.0	350.0	0.00
16	Male	22	27.4	1634.4	2599.7	21.9	10.9	0.20	379.2	1.86	400.0	0.0	416.7	21.1	3.46
17	Male	46	26.2	818.1	4265.3	88.8	27.1	1.22	478.7	1.52	336.7	189.3	501.3	116.9	18.37
18	Male	38	26.3	588.2	2282.8	222.4	15.2	0.65	117.0	0.77	70.2	0.0	296.2	157.0	6.15
19	Male	41	28.9	2235.7	4667.8	206.8	57.2	0.24	837.4	2.85	957.3	0.0	728.6	816.6	20.42
20	Male	35	26.8	266.5	578.1	397.9	10.3	0.49	13.5	0.53	0.0	0.0	282.8	100.0	0.84
21	Female	61	26.5	1131.9	3607.1	185.8	15.8	0.40	262.6	4.38	429.0	0.0	388.7	750.5	24.05
22	Male	56	25.8	229.3	1054.4	141.4	9.8	0.59	56.2	0.18	111.1	0.0	359.1	83.3	1.70
23	Male	71	24.9	256.2	612.1	527.0	47.6	0.45	28.9	0.41	0.0	0.0	494.1	158.8	0.00

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24	Male	40	25.5	268.2	915.1	510.9	13.9	0.28	41.3	0.20	20.7	0.0	279.8	111.4	0.15
25	Male	45	23.6	228.8	985.3	134.9	27.0	0.48	23.0	0.57	15.2	0.0	293.2	98.0	1.07
26	Male	61	26.1	198.3	772.6	465.7	12.2	0.30	12.5	0.30	3.7	61.6	597.0	391.8	1.04
27	Male	83	26.8	1164.0	2016.0	362.3	10.2	0.66	760.3	4.29	219.9	0.0	744.7	780.1	2.68
28	Female	45	28.0	2167.4	2766.1	168.5	5.2	0.13	390.6	1.86	681.5	0.0	407.4	477.8	4.55
29	Female	69	27.2	1401.8	2923.4	256.6	14.8	0.31	822.4	1.61	513.9	0.0	557.3	379.9	8.68
30	Male	52	25.7	238.3	477.4	268.2	14.7	0.47	36.2	0.46	0.0	0.0	369.8	494.1	2.07
31	Male	30	22.0	98.2	50.5	302.8	5.2	0.34	26.4	0.26	183.2	0.0	68.1	41.9	10.25
32	Female	24	30.7	3568.5	6685.1	1697.6	15.3	0.13	578.0	8.12	1576.9	0.0	1043.3	566.3	12.59
33	Female	67	9.0	55480.8	4417.0	2576.3	1.8	0.51	466.1	15.41	969.6	0.0	93.2	96.9	1.63
34	Male	40	28.4	3919.7	2381.0	2380.9	0.0	0.00	205.6	1.19	0.0	0.0	166.7	142.9	0.00
35	Female	50	14.8	40219.1	6010.6	915.6	30.8	0.13	461.2	4.91	1283.8	2883.1	376.0	80.3	0.64
36	Female	38	28.7	5192.6	3571.4	1870.4	0.0	0.00	622.4	1.14	0.0	0.0	535.7	285.7	0.00
37	Female	27	27.4	1086.1	1227.4	406.1	14.2	0.44	324.8	1.30	740.9	0.0	642.3	102.2	7.05
38	Male	34	25.2	135.1	1405.7	410.3	18.6	0.17	56.9	0.37	0.0	0.0	112.5	137.5	2.48
39	Female	58	20.5	1401.2	1905.3	347.5	14.8	0.12	543.7	2.30	502.6	0.0	280.2	434.4	8.95
40	Male	31	27.3	2753.5	2237.4	299.2	17.2	0.28	485.1	2.24	1450.0	0.0	515.8	205.3	4.82
41	Female	73	31.1	2072.4	2650.3	609.8	7.8	0.31	635.3	5.59	862.3	0.0	1108.7	992.8	6.27
42	Male	53	25.5	1935.4	3251.6	304.3	10.8	0.30	508.1	1.85	1625.9	39.6	243.8	407.6	3.74
43	Male	39	28.0	1297.5	2711.4	294.5	25.9	0.55	620.2	9.53	502.7	0.0	827.9	532.8	10.67
44	Male	59	9.4	63.4	737.2	263.3	17.7	1.72	7.3	0.12	0.0	26.7	273.4	58.4	0.30
45	Male	46	25.3	455.2	3225.3	173.8	21.1	1.84	234.5	0.96	393.8	0.0	973.4	584.3	11.06
46	Female	57	27.4	1978.0	2607.5	438.1	9.7	0.34	721.3	2.44	728.4	0.0	500.0	290.1	12.58
47	Male	68	0.3	8.1	108.8	221.3	5.5	1.94	1.4	0.08	5.3	85.3	85.5	11.4	0.00

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48	Male	79	27.7	1809.9	3559.6	576.2	62.4	0.07	758.5	3.35	1173.4	0.0	1391.1	1100.8	7.26
49	Male	41	27.5	13499.9	8966.4	946.3	54.9	0.17	2678.0	13.54	1781.4	0.0	390.1	1524.9	25.78
50	Male	20	28.8	3183.3	4534.6	1092.1	19.6	5.51	1196.5	3.14	989.4	0.0	676.1	433.1	9.17
51	Male	44	26.1	235.1	604.1	388.8	12.4	0.72	20.8	0.23	204.5	0.0	513.7	58.4	2.75
52	Male	58	13.5	95.4	254.5	335.5	6.0	1.19	30.6	0.48	135.9	0.0	228.1	145.2	0.22
53	Male	40	26.0	573.1	1194.6	217.7	23.0	0.08	232.5	1.85	87.3	0.0	234.9	84.3	8.29
54	Male	45	26.9	178.3	1020.4	727.4	15.8	0.49	25.3	0.33	0.0	0.0	357.1	71.4	2.29
55	Male	34	24.5	495.1	29.9	434.5	8.2	0.11	161.1	1.39	92.7	0.0	141.5	22.0	2.19
56	Male	36	24.2	307.4	1259.5	725.5	191.4	0.43	79.7	0.42	0.0	3597.4	651.3	161.5	2.31
57	Female	46	26.0	306.7	1113.8	430.4	10.6	0.57	84.7	0.37	69.0	0.0	381.2	172.4	3.57
58	Male	72	25.8	433.2	1379.9	306.4	3.0	0.56	34.5	0.19	16.1	0.0	730.6	80.6	0.75
59	Male	52	29.1	133.6	1020.4	868.3	10.3	0.00	115.2	0.50	0.0	0.0	255.1	40.8	0.00
60	Male	38	54.4	2181.4	16666.7	25475.6	0.0	0.00	271.2	3.67	0.0	0.0	333.3	166.7	0.00
61	Male	38	27.9	1190.6	2043.1	354.3	18.3	0.11	423.6	1.58	367.3	4247.4	494.9	584.2	12.07
62	Male	35	24.6	296.2	425.0	132.4	271.0	4.46	365.1	12.81	202.8	0.0	111.3	82.5	2.68
63	Female	48	32.3	420.7	2777.8	1606.9	2.5	0.00	465.2	4.44	20694.4	0.0	222.2	277.8	0.00
64	Female	66	25.4	128.3	980.4	818.1	23.6	0.45	19.9	0.29	343.1	0.0	264.7	98.0	0.00
65	Male	45	27.3	1595.9	2807.9	197.1	19.5	1.92	842.1	1.89	265.6	0.0	593.8	468.8	14.02
66	Male	42	23.7	404.5	1158.4	165.1	8.8	0.85	24.0	0.49	35.6	0.0	514.4	150.0	1.03

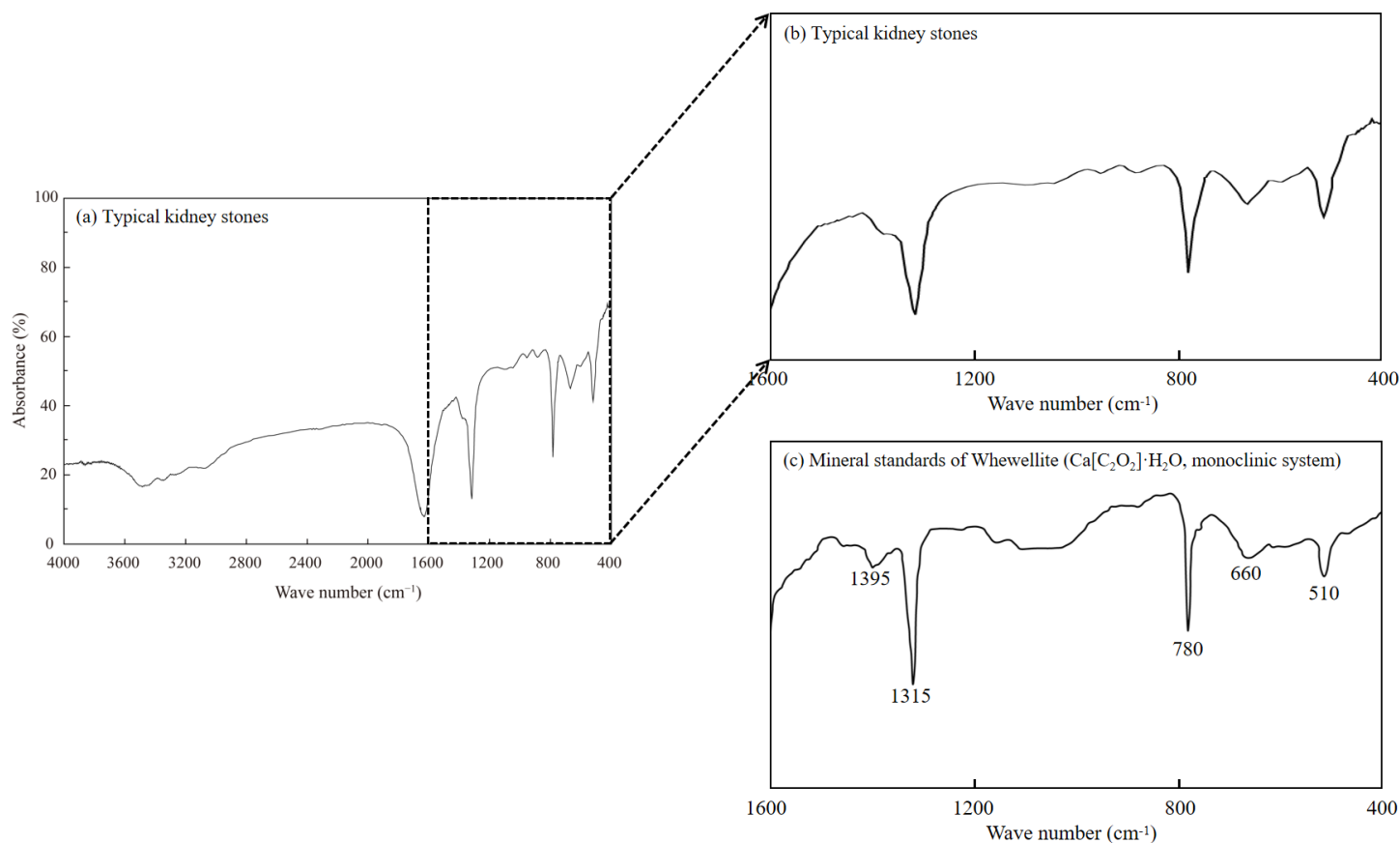


Figure S1. The comparison of infrared spectrum of (a, b) typical kidney stones and (c) mineral standards of Whewellite (Calcium oxalate monohydrate, $\text{Ca}[\text{C}_2\text{O}_2]\cdot\text{H}_2\text{O}$, monoclinic system). As shown in (c), the sharp absorption bands were observed at 1315 cm^{-1} , 780 cm^{-1} , 510 cm^{-1} and the relatively weak absorption bands were observed at 1395 cm^{-1} , 660 cm^{-1} (Mineral Infrared Spectrum Atlas, 1982, Science Press: Beijing). The similar sharp absorption bands and the relatively weak absorption bands were also found in the typical kidney stones sample in (b), which characterize the mineralogical compositions of sample. For example, C-O stretching attributes to the band at $\sim 1315\text{ cm}^{-1}$, the bands at ~ 780 and $\sim 660\text{ cm}^{-1}$ were the result of C-H bending together with the out of plane O-H bending.

Text S1. The information of instrument and the parameters of infrared spectroscopy analysis system (LIIR-20, Lambda scientific, China)

Spectrum range: 4000 cm^{-1} to 400 cm^{-1}

Resolution: 1.5 cm^{-1}

Transmittancy repeatability: $<0.5\%$

Signal to noise ratio: >15000

Baseline straightness: $\pm 1\%$

Detector: Deuterium triglyceride sulfate crystal (DTGS)

Light source: Infrared light supply