

SUPPLEMENTARY INFORMATION FOR:

Morpho-Constitutional Classification of Urinary Stones as Prospective Approach for the Management of Human Pathological Biomineralization: New Insights from Southern Italy

Francesco Izzo ¹, Alessio Langella ¹, Chiara Germinario ², Celestino Grifa ², Ettore Varricchio ², Maria Chiara Di Meo ², Luigi Salzano ³, Giuseppe Lotrecchiano ³ and Mariano Mercurio ^{2,*}

¹ Department of Earth Sciences, Environment and Resources, University of Naples Federico II, Via Cintia, 80126 Naples, Italy

² Department of Science and Technology, University of Sannio, Via de Sanctis snc, 82100 Benevento, Italy

³ UOC Urology, San Pio Hospital, Via dell'Angelo, 82100 Benevento, Italy

* Correspondence: mariano.mercurio@unisannio.it

Table S1. Analytical techniques applied for the characterization of human urinary stones. Note: SM, stereomicroscopy; PLM, polarized light microscopy; scanning electron microscopy; FTIR, Fourier transform infrared spectroscopy.

n.	ID Sample	SM	PLM	SEM	FTIR
1	KS001	x			x
2	KS002	x			x
3	KS003	x			x
4	KS004	x	x		x
5	KS005	x			x
6	KS006B	x	x	x	x
7	KS007	x	x		x
8	KS008	x	x	x	x
9	KS009	x			x
10	KS010	x			x
11	KS011B	x	x		x
12	KS012B	x	x		x
13	KS013	x	x	x	
14	KS014	x	x		x
15	KS015	x			x
16	KS016	x	x		x
17	KS017	x			x
18	KS018	x			x
19	KS020B	x	x		x
20	KS021	x			x
21	KS022B	x	x		x
22	KS023B	x	x		x
23	KS024	x			x
24	KS025	x			x
25	KS026	x	x		x
26	KS027	x		x	x
27	KS028B	x		x	x
28	KS029B	x			x
29	KS030	x	x	x	x
30	KS031	x	x		x
31	KS032B	x		x	x
32	KS033B	x			x
33	KS034B	x			x
34	KS035B	x			x
35	KS036B	x			x
36	KS037B	x			x
37	KS038B	x			x
38	KS039	x		x	x
39	KS040	x			x
40	KS041	x		x	x
41	KS043	x			x
42	KS044	x		x	x
43	KS045	x			x
44	KS046	x			x
45	KS047	x			x
46	KS048	x			x
47	KS049	x			x
48	KS050B	x			x
49	KS051B	x			x

Table S2a - FTIR data for CaOx urinary stones (wavenumbers expressed in cm⁻¹).

KS001	KS004	KS005	KS010	KS012B	KS014	KS017	KS018	KS021	KS024	KS025	KS026	KS027	KS028B	KS030	KS031	KS033B	KS036B	KS040	KS044	KS045	KS048	KS049	KS051	Average	Chemical phases
3428	3425	3444	3426	3440	3423	3429	3427	3446	3428	3429	3427	3427	3462	3429	3428	3427	3439	3426	3425	3423	3462	3423	3427	3432	Calcium Oxalate
3325	3337	3336	3324	3318	3326	3335	3324	3327	3337	3328	3332	3325	3325	3323	3335	3329	3324	3338	3330	3336	3349	3331	3337	3331	Calcium Oxalate
3246	3245	3235	3245	3225	3248	3234	3232	3225	3233	3240	3246	3247	3246	3240	3248	3244	3236	3240	3246	3248	3242	3243	3245	3241	Calcium Oxalate
3057	3047	3047	3044	3043	3049	3051	3042	3014	3050	3047	3044	3044	3087	3053	3041	3047	3054	3044	3044	3045	3092	3056	3048	3050	Calcium Oxalate
			-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2953	-	-	-	2953	Organic matter
	2931	2938	-	-	-	2938	-	2822		2934	-	-	-	-	-	-	2928	-	2934	2916	2920	2929	-	2919	Organic matter
			-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2848	2841	2850	-	2846	Organic matter
			-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1733	-	-	-	1733	Organic matter
1612	1610	1615	1610	1610	1611	1612	1612	1612	1615	1613	1611	1611	1618	1609	1613	1610	1615	1615	1612	1611	1615	1608	1612	1612	Calcium Oxalate
			-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1472	1473	-	-	1472	Calcium Phosphate/Organic matter
			-	-	-	-	-	1437	-	-	-	-	-	-	-	-	-	-	-	1463	-	-	-	1450	Calcium Phosphate/Organic matter
1364	1380	1367	1367	1380	1367	1366	1380	1381	1379	1368	1366	1368		1367	1379	1367		1368	1374	1377	-	1380	1368	1372	Calcium Oxalate
1315	1313	1315	1313	1313	1314	1314	1314	1313	1314	1314	1314	1313	1320	1313	1314	1313	1316	1313	1313	1313	1318	1313	1313	1314	Calcium Oxalate
			-	-	-	-	-	1123	-	-	-	-	-	-	-	-	-	-	1124	-	-	-	-	1123	Uric acid
1044	1053	1067	1095	1044	1100	1096	1038	1027	1079	1081	1090	1111	1034	1096	1087	1087	1101	1088	-	1069	1037	1096	1063	1073	Calcium Phosphate
			-	-	-	-	-	992	-	-	-	-	-	-	-	-	-	-	992	-	-	1013	-	999	Uric acid
947	946	949	947	952	947	948	949	948	948	946	947	947	914	948	948	946	-	947	948	953	959	945	949	947	Calcium Oxalate
915			-	-	-	-	-	-	-	-	-	-	-	-	-	-	913	-	-	-	914	-	-	914	Calcium Phosphate
884	878	884	884	886	885	884	883	880	884	885	885	885		885	884	885		886	885	886	886	863	885	883	Calcium Oxalate
779	779	779	779	779	779	779	779	779	779	779	779	779	779	779	779	779	779	779	779	779	780	779	779	779	Calcium Oxalate
			-	-	-	-	-	745	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	Uric acid
646	658	659	657	656	658	657	658	653	659	657	658	656	-	656	659	656	-	660	657	654	-	659	664	657	Calcium Oxalate
600	601	601	597	597	595	598	600	619	598	599	597	596	602	596	596	596	603	603	594	591	602	599	600	599	Calcium Oxalate
			-	-	-	-	-	574	-	-	-	-	-	-	-	-	-	-	-	-	563	-	574	-	Calcium Phosphate/Uric acid
513	513	513	514	511	513	513	513	514	515	513	513	513	514	512	514	513	513	513	514	513	514	512	513	513	Calcium Oxalate
			-	-	-	-	-	475	-	-	-	421	-	-	-	-	-	-	-	-	-	-	-	-	Uric acid

Table S2b - FTIR data for UA urinary stones (wavenumbers expressed in cm⁻¹).

KS003	KS009	KS011B	KS015	KS016	KS020B	KS022B	KS023B	KS029B	KS034B	KS035B	KS037B	KS038B	KS039	KS046	KS050B	Average	Chemical phases
-	-	-	3436	-	-	-	-	-	-	-	3446	-	3444	-	-	3442	Calcium Oxalate
-	-	-	-	-	-	-	-	-	-	-	-	-	3322	-	-	3322	Calcium Oxalate
3090	3078	3089	3089	3088	3084	3082	3088	3082	3099	3089	3079	3095	3089	3101	3082	3088	Uric acid
2991	2992	2992	3000	2998	2996	2992	3005	2991	3000	2999	2994	2991	2994	2992	2991	2995	Uric acid
2917	2914	2918	2918	2918	2912	2914	2917	2920	2926	2915	2915	2923	2924	2912	2916	2917	Uric acid
-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2847	2847	Organic matter
-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2818	2818	Organic matter
2789	2788	2788	2808	2814	2785	2787	2793	2788	2792	2794	2787	2785	2802	2779	2792	2792	Uric acid
2692	2694	2687	2695	2692	2680	2687	2684	2693	2693	2689	2697	2690	2693	2689	2689	2690	Uric acid
2606	2606	2605	2606	2606	2609	2600	2603	2606	2598	2605	2605	2602	2605	2606	2604	2605	Uric acid
1659	1656	1661	1662	1661	1654	1662	1662	1660	1664	1654	1654	1654	1652	1654	1661	1658	Uric acid
1584	1584	1584	1586	1585	1585	1584	1585	1585	1586	1584	1586	1584	1587	1577	1585	1584	Uric acid
1483	1483		1484	1484	1490	1485	1485	1484	1490	1490	1489	1482	1486	1483	1485	1486	Uric acid
1434	1434	1435	1435	1434	1434	1435	1435	1434	1436	1436	1436	1435	1436	1433	1435	1435	Uric acid
1399	1399	1398	1400	1399	1399	1399	1399	1399	1399	1399	1398	1398	1399	1405	1398	1399	Uric acid
1347	1347	1347	1348	1347	1347	1347	1347	1347	1348	1348	1348	1347	1348	1349	1348	1348	Uric acid
1301	1301	1301	1309	1302	1302	1301	1302	1301	1302	1303	1310	1301	1311	1301	1301	1303	Uric acid/Calcium oxalate
1223	1223	1223	1225	1223	1224	1223	1223	1223	1222	1223	1223	1222	1228	1218	1223	1223	Uric acid
1120	1120	1121	1121	1121	1121	1121	1121	1120	1121	1120	1121	1120	1122	1112	1121	1120	Uric acid
1025	1025	1025	1025	1025	1026	1025	1026	1025	1026	1026	1025	1025	1026	1025	1026	1025	Uric acid
990	989	990	990	990	990	990	990	990	990	989	990	990	991	985	990	990	Uric acid
875	875	875	876	875	876	875	875	875	876	876	876	875	876	876	875	875	Uric acid
778	778	779	778	779	781	779	780	778	780	780	779	778	778	783	779	779	Uric acid
742	742	742	743	742	743	742	743	741	743	743	743	742	744	744	743	743	Uric acid
703	703	703	704	703	702	703	703	703	704	702	703	703	704	699	703	703	Uric acid
616	616	617	617	616	617	617	617	616	617	616	617	616	617	614	617	616	Uric acid
571	571	572	572	572	572	571	572	572	572	571	572	571	573	570	572	572	Uric acid
519	519	519	518	519	519	520	520	519	520	515	518	511	517	512	520	518	Uric acid
470	470	470	471	470	471	469	470	470	470	470	470	469	471	468	470	470	Uric acid

Table S2c - FTIR data for CaP urinary stones (wavenumbers expressed in cm⁻¹).

KS006B	KS008	Chemical phases
3542	-	Brushite
3474	-	Brushite
-	3292	Carbonated apatite/Calcium oxalate
3268	-	Brushite
3155	-	Brushite
1644	-	Brushite
-	1621	Calcium oxalate
-	1461	Carbonated apatite
-	1421	Carbonated apatite
1323	1317	Calcium oxalate
1205	-	Brushite
1135	-	Brushite
-	1026	Carbonated apatite
1059	-	Brushite
986	962	Carbonated apatite/Brushite
872	878	Carbonated apatite/Brushite
784	780	Brushite/Calcium oxalate
655	666	Brushite/Calcium oxalate
-	601	Carbonated apatite
577	-	Brushite
-	561	Carbonated apatite
523	-	Brushite

Table S2d - FTIR data for mixed urinary stones (wavenumbers expressed in cm⁻¹).

KS002	KS039	KS041	KS007	KS032B	KS047	Average	Chemical phases
3426	3444	3460	3426	3460	3428	3441	Calcium Oxalate
3325	3322	-	3337	-	3336	3330	Calcium Oxalate
-	-	-	3247	3306	3256	3270	Calcium Oxalate
-	-	-	3049	-	3046	3048	Calcium Oxalate
3011	3089	3013	-	-	-	3038	Uric acid
-	2994	2898	-	-	-	2946	Uric acid
-	2924	-	-	-	2919	2922	Uric acid/Organic matter
2822	2802	2803	-	-	2848	2819	Uric acid/Organic matter
2689	2693	2673	-	-	-	2685	Uric acid
2606	2605	-	-	-	-	2606	Uric acid
1655	1652	1631	-	-	-	1646	Uric acid
1617	-	-	1613	1616	1615	1615	Calcium Oxalate
-	1587	1591	-	-	-	1589	Ammonium urate/Uric acid
-	-	1540	-	-	-	1540	Ammonium urate
-	1486	-	-	-	-	1486	Uric acid
1435	1436	1430	-	-	-	1433	Uric acid
1399	1399	1386	-	-	-	1395	Uric acid
1348	1348	1341	-	-	-	1346	Uric acid
1313	1311	1315	1314	1319	1313	1314	Calcium Oxalate
-	-	1273	-	-	-	1273	Ammonium urate
1229	1228	-	-	-	-	1228	Uric acid
-	-	1138	-	-	-	1138	Ammonium urate
1122	1122	1124	-	-	-	1123	Uric acid
1026	1026	1027	1038	1031	1036	1030	Uric acid/Calcium phosphate
-	-	1003	-	-	-	1003	Ammonium urate
-	991	-	-	963	949	968	Uric acid/Calcium phosphate
-	-	-	951	-	-	951	Calcium Oxalate
-	-	-	-	913	-	913	Calcium phosphate
877	876	883	882	-	884	880	Calcium Oxalate/Uric acid
779	778	780	779	778	779	779	Calcium Oxalate/Uric acid
-	-	768	-	-	-	768	Ammonium urate
744	744	744	-	-	-	744	Uric acid
704	704	-	-	-	-	704	Uric acid
-	-	722	-	-	-	722	Ammonium urate
655	-	635	659	-	661	652	Calcium Oxalate
-	617	597	-	-	-	607	Ammonium urate/Uric acid
-	-	-	601	603	603	603	Calcium phosphate
573	573	-	571	563	565	569	Uric acid/Calcium phosphate
517	517	522	513	515	514	516	Calcium Oxalate/Uric acid
473	471	487	-	-	-	477	Uric acid

Table S3 - Average concentration of major (>1 wt.%, in bold) and trace elements (<1wt.%) detected for urinary stones by EDS.

Sample ID	Mineral phases	Ca	P	S	Na	Zn	Mg	Al	Si	Cl
KS013	Ca-Oxalates	28.66								
	Ca-Oxalates	26.31	0.21	0.08						
	Ca-Oxalates	25.08	0.08							
	Ca-Oxalates	24.37	0.13	0.10						
	Ca-Oxalates	26.63								
	Ca-Oxalates	28.09		0.13						0.08
	Ca-Oxalates	24.16	0.35	0.31						
	Ca-Oxalates	24.50	0.37	0.31						
	Ca-Oxalates	24.93	0.38	0.29					0.04	
	Ca-Oxalates	25.40	0.33	0.31						
	Ca-Oxalates	24.35	0.26	0.25						
	Ca-Oxalates	24.81	0.25	0.35						
	<i>Average</i>	25.61	0.26	0.24					0.04	0.08
	<i>σ</i>	1.50	0.11	0.10						
KS028B	Ca-Oxalates	27.87	0.06							
	Ca-Oxalates	31.56	0.10	0.09						
	Ca-Oxalates	29.34								
	Ca-Oxalates	32.76								
	Ca-Oxalates	27.95		0.10						0.08
	Ca-Oxalates	26.94	0.13							
	Ca-Oxalates	31.13								0.08
	Ca-Oxalates	29.22								0.06
	<i>Average</i>	29.60	0.10	0.10						0.07
	<i>σ</i>	2.04	0.04	0.01						0.01
KS008	Ca-Oxalates	26.21								
	<i>Average</i>	26.21								
	<i>σ</i>	-								
	Ca-Phosphates	31.79	17.60		0.90		0.84			
	Ca-Phosphates	28.60	15.39		0.80		0.63			0.28
	Ca-Phosphates	27.74	14.00		0.57		0.51			-
	Ca-Phosphates	31.51	17.34		0.83	0.18	0.89			0.19
	Ca-Phosphates	31.51	17.49		1.00	0.17	0.86			-
	<i>Average</i>	30.23	16.36		0.82	0.18	0.75			0.24
	<i>σ</i>	1.91	1.60		0.16	0.01	0.17			0.06