Supplementary Material for

Analysis of Human Kidney Stones Using Advanced Characterisation Techniques

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Figure S1. TGA (—) and DSC (—) curves for kidney stone samples M5 and M6 in the oxygen atmosphere.

Figure S2. Elemental analysis (EDX) of kidney stone samples a) M1, b) M5, c) M6, d) F6. The peak height (cps/eV) represents a relative abundance of detected elements in the sample.

Figure S3. TGA (—) and DSC (—) curves for kidney stone sample F4 and F5 in the oxygen atmosphere.

Figure S4. Elemental analysis (EDX) of kidney stone F8. The peak height (cps/eV) represents a relative abundance of detected elements in the sample.

Figure S5. IR spectra of two samples of calcium phosphate kidney stone F2 and M2. Data collected using DRIFT technique. Samples (5 mg) were mixed with spectroscopy grade KBr (100 mg) before analysis. Characteristic bands are labelled at observed wavenumber.

Figure S6. PXRD patterns of the two stone samples (F2 and M2) compared with literature data for weddellite (*wd*), struvite (*s*) and apatite (*a*) [43, 48].

Figure S7. TGA (—) and DSC (—) curves for kidney stone sample F1 (a), M2 (b), and M7 (c) in the oxygen atmosphere.

Figure S8. Elemental analysis (EDX) of kidney stone samples a) F1, b) F2, c) M2, and d) M4. The peak height (cps/eV) represents a relative abundance of detected elements in the sample.

Figure S9. Elemental analysis (EDX) of kidney stone sample F7. The peak height (cps/eV) represents a relative abundance of detected elements in the sample.

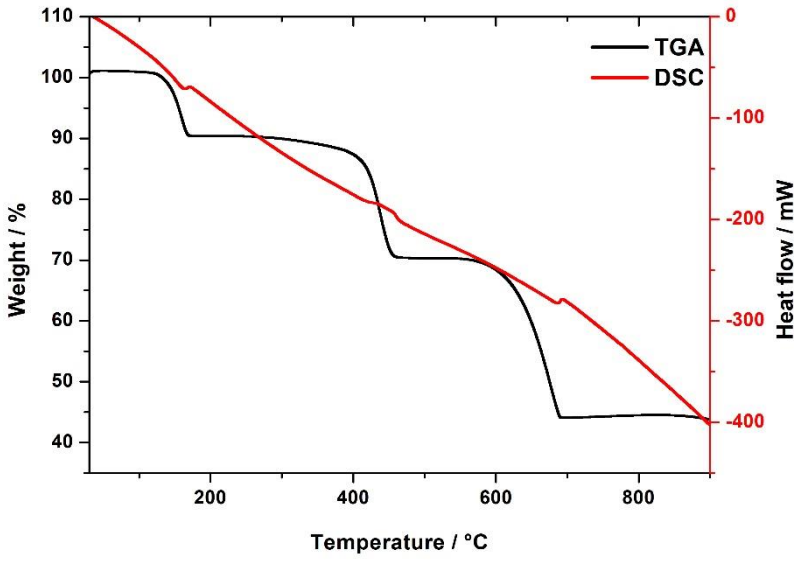
Table S1.

Sample (patient year of birth)	Stone type (composition)	*a*	*s*	*w*	*wd*	*b*	*u*	*c*	Rietveld refinement parameters		
									R_p	R_{wp}	R_{exp}
M1 (1971)	mostly calcium oxalate (*w*)			90	10				10.8195	10.9182	4.0566
M3 (1984)		8		24	68				7.0961	10.3137	4.2026
M5 (1964)				99					8.4317	12.3511	3.8988
M6 (1965)				99					5.8497	9.3351	4.1518
F6 (1972)				98					7.4515	12.7517	4.0238
F8 (1990)	mixed calcium oxalate (*w*, *wd*) + calcium phosphate (*a*)	16		51	32				9.0442	13.6340	3.4817
F4 (2001)		34		20	46				11.6239	17.7983	3.7207
F5 (1988)		12		68	19				7.5011	10.7684	3.9511
F1 (1976)	mostly calcium phosphate (*a*, *s*, *b*) + some *wd*	82	15		3				8.4019	12.5616	3.7906
F2 (1994)		62	27		11				4.9206	7.0567	3.3918
F3 (1959)		95	5						8.8802	12.4724	3.9217
M2 (2007)		80	20						10.8195	16.5292	4.2888
M4 (1972)		37	51		11				7.3289	9.9661	3.7949
M7(1965)		51			10	38			7.5144	10.7147	4.0278
F7 (1956)	mixed uric acid (*u*) + (*w*)			54			45		20.0555	29.3140	3.3014
M8 (2008)	mixed cystine (*c*) + phosphate (*s*)		18					82	28.9990	41.5202	3.6321

a – apatite (hydroxyapatite)
s – struvite
w – whewellite
wd – weddellite
u – uric acid
b - brushite
c – cystine

Figure S1.

(A)



(B)

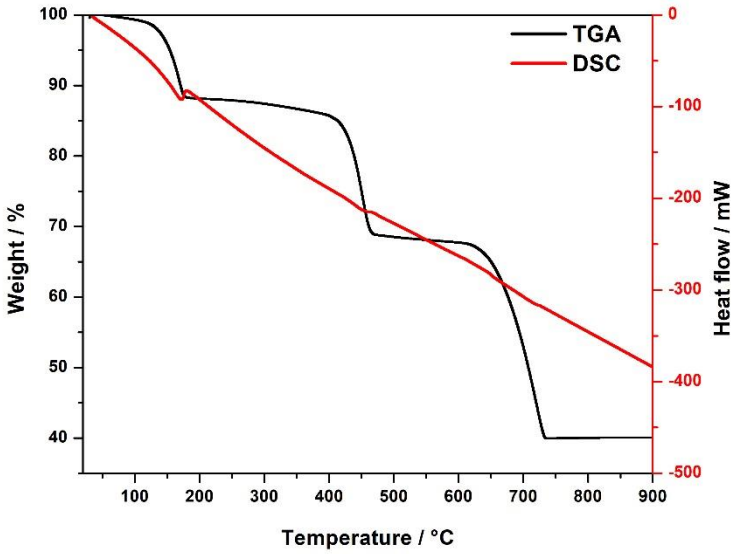
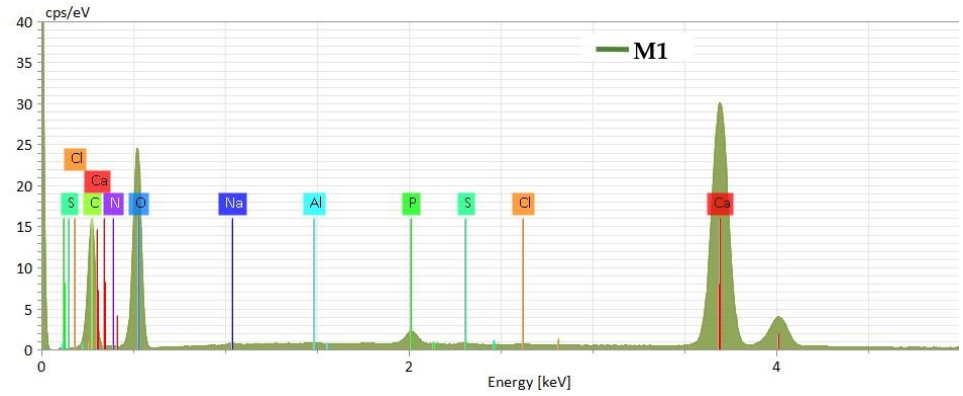
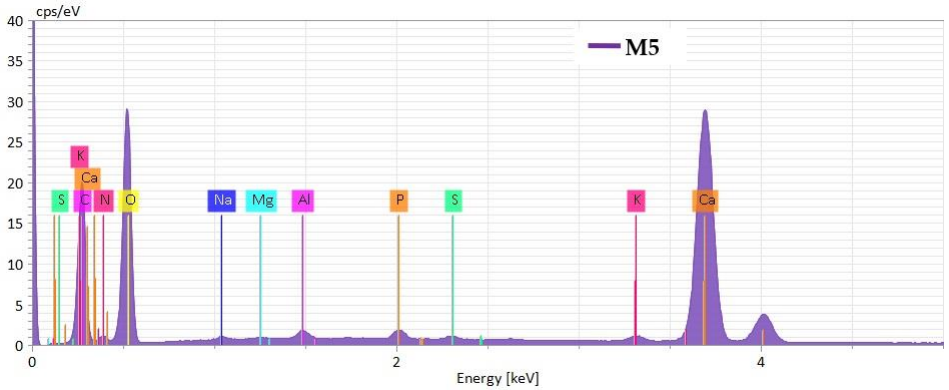


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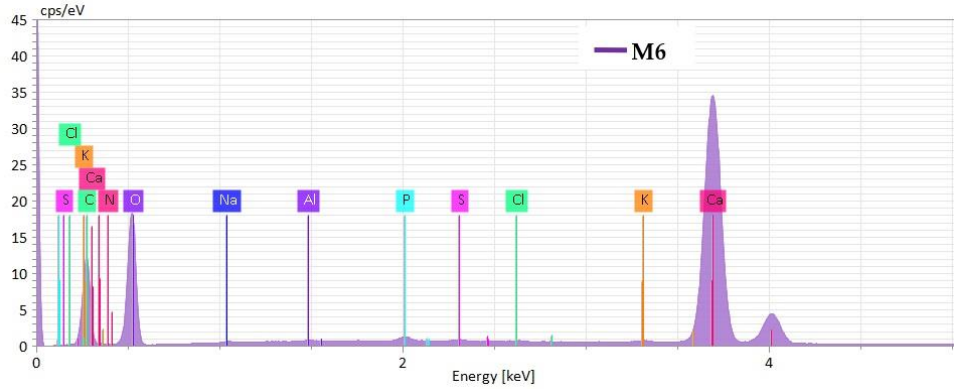
(A)



(B)



(C)


cps/eV
M6
Cl
K
Ca
S
C
N
O
Na
Al
P
S
Cl
K
Ca
Energy [keV]

(D)

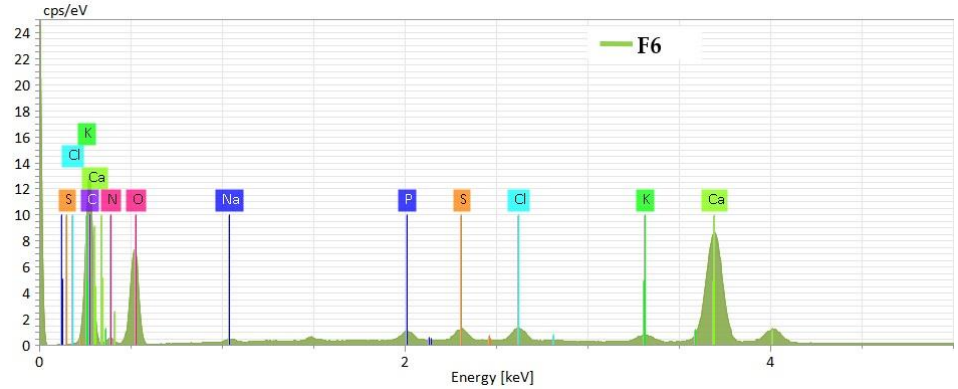
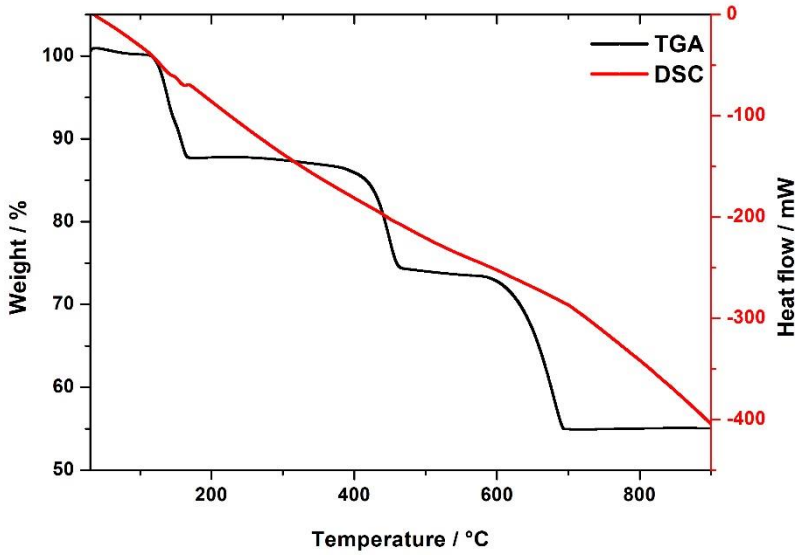

cps/eV
F6
K
Cl
Ca
S
C
N
O
Na
P
S
Cl
K
Ca
Energy [keV]

Figure S3.

(A)


TGA
DSC
Weight / %
Heat flow / mW
Temperature / °C
100
90
80
70
60
50
0
-100
-200
-300
-400
200
400
600
800

(B)

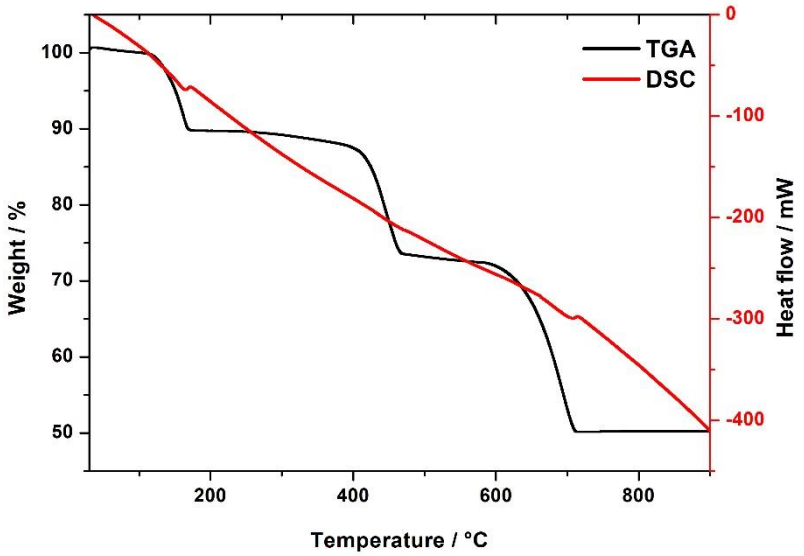

TGA
DSC
Weight / %
Heat flow / mW
Temperature / °C
100
90
80
70
60
50
0
-100
-200
-300
-400
200
400
600
800

Figure S4.

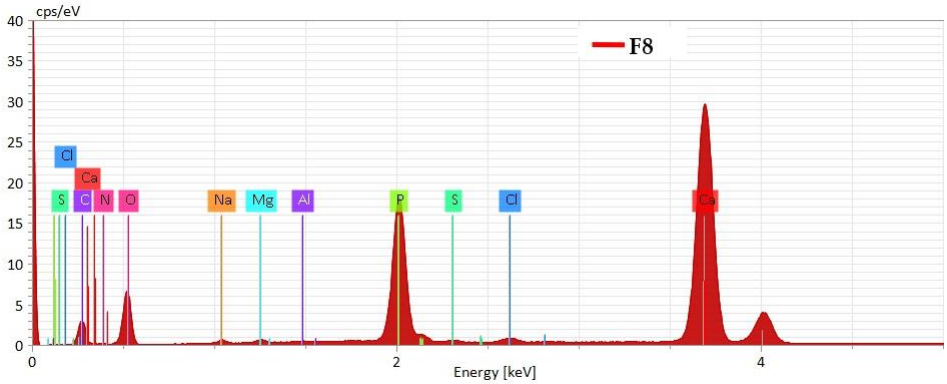


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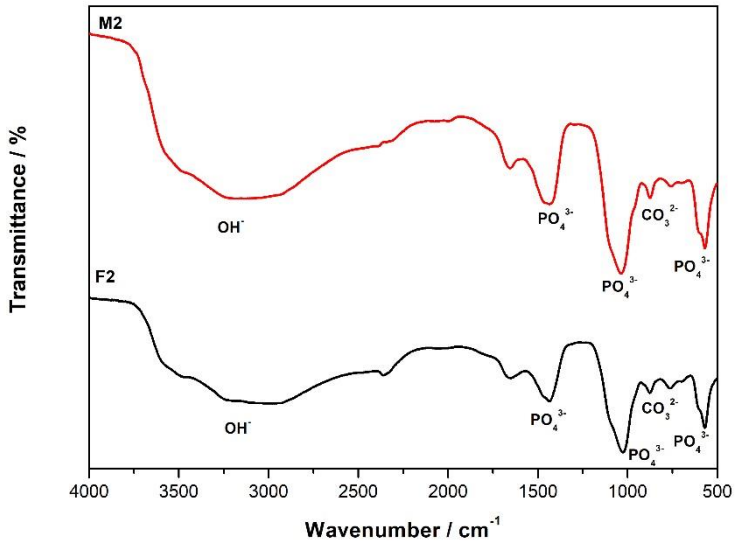


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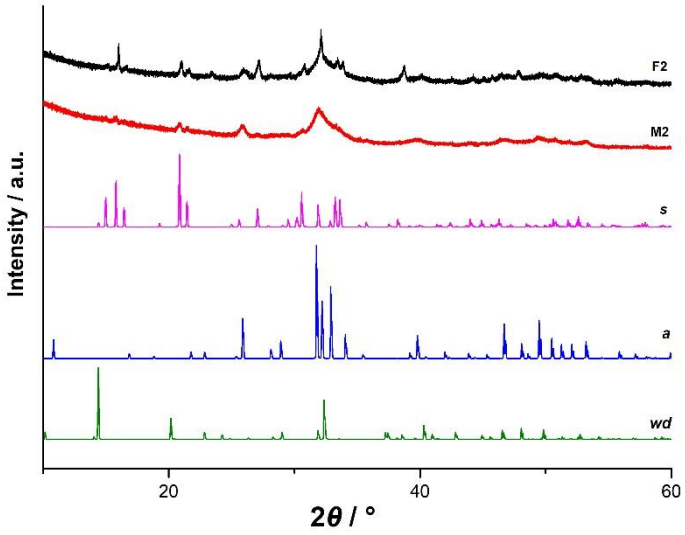
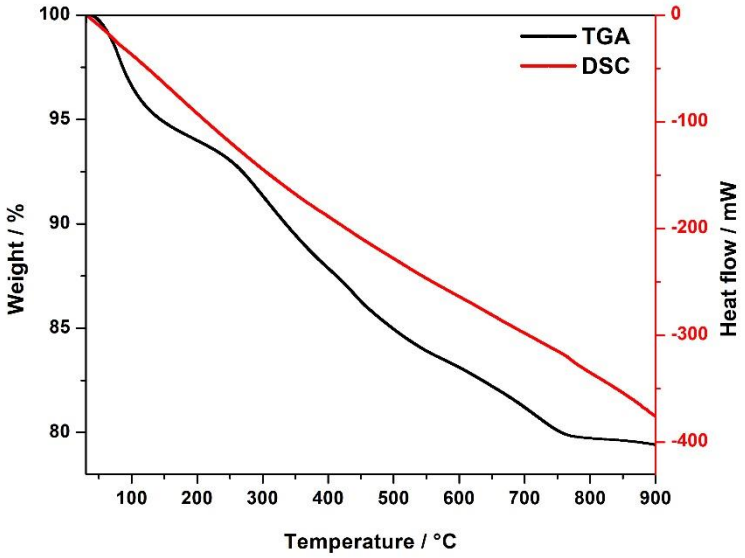
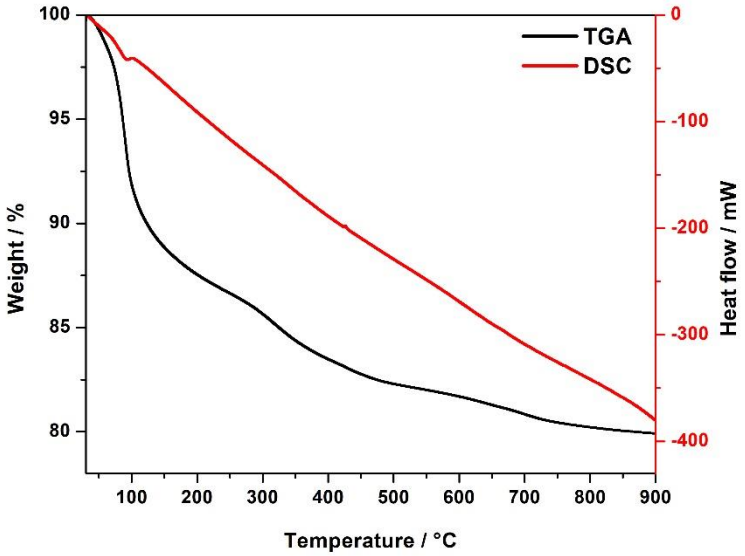


Figure S7.

(A)



(B)


TGA
DSC
Weight / %
Heat flow / mW
Temperature / °C
100
95
90
85
80
0
-100
-200
-300
-400
100
200
300
400
500
600
700
800
900

(C)

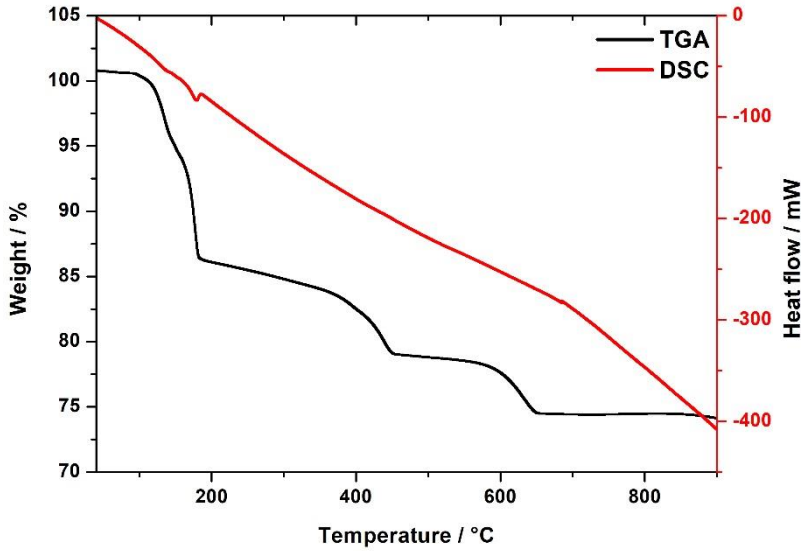
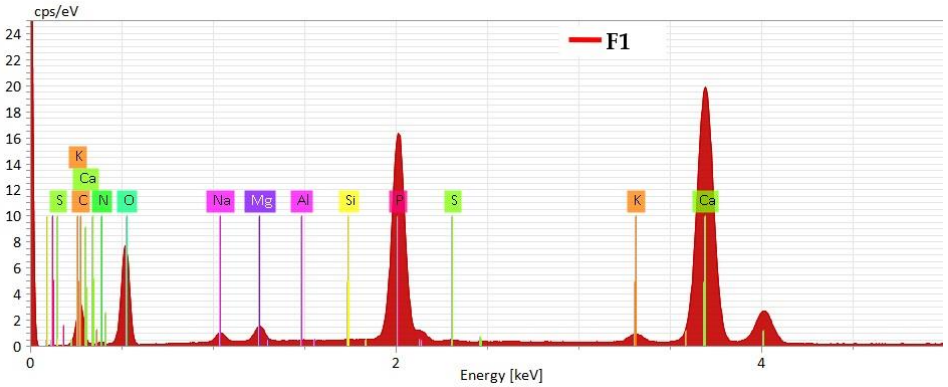
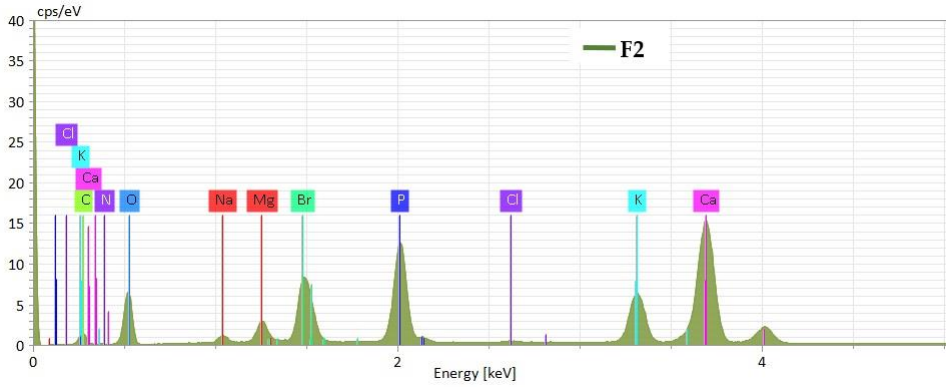

TGA
DSC
Weight / %
Heat flow / mW
Temperature / °C
105
100
95
90
85
80
75
70
0
-100
-200
-300
-400
200
400
600
800

Figure S8.

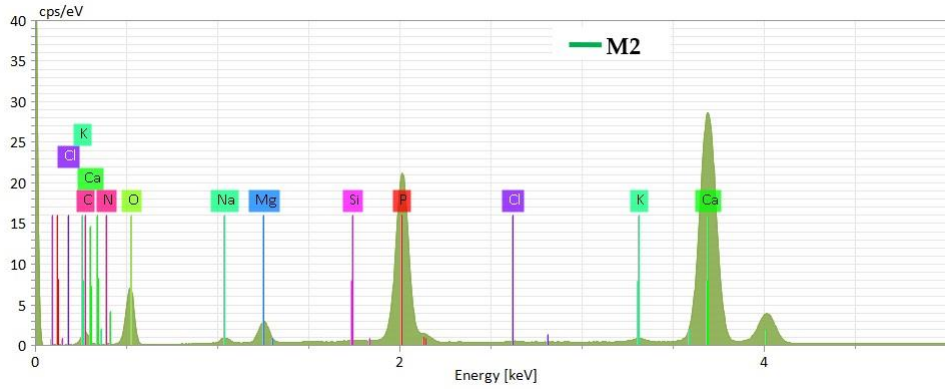
(A)



(B)



(C)



(D)

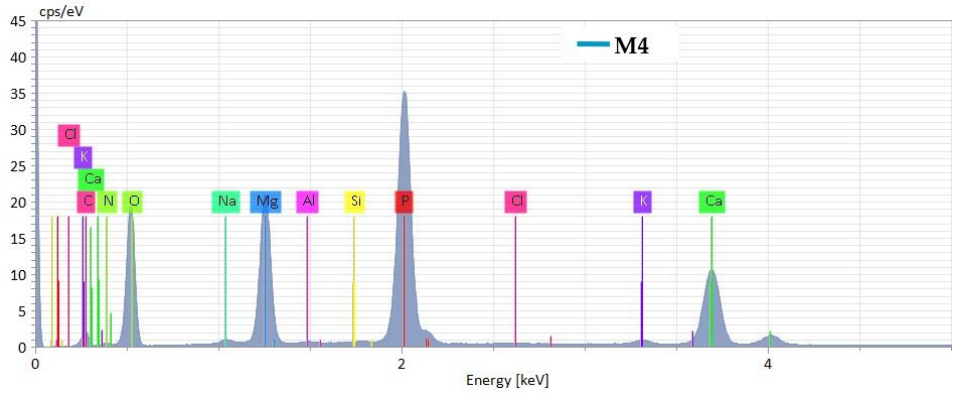
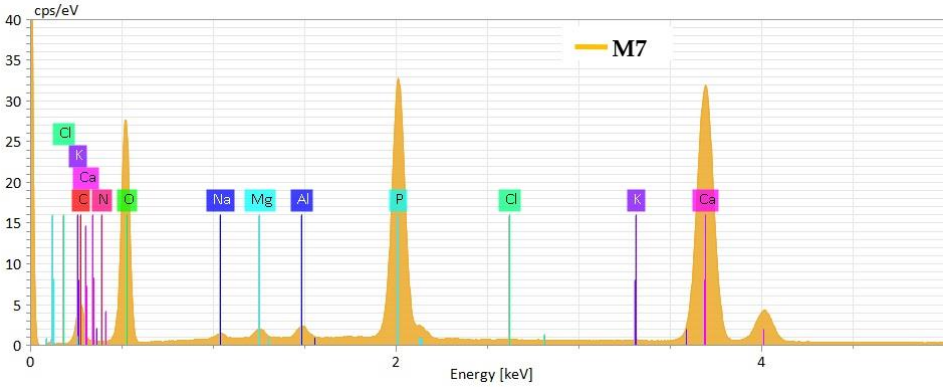

cps/eV
M4
Cl
K
Ca
C
N
O
Na
Mg
Al
Si
P
Cl
K
Ca
Energy [keV]

Figure S9.


cps/eV
M7
Cl
K
Ca
C
N
O
Na
Mg
Al
P
Cl
K
Ca
Energy [keV]