Electronic Supplementary Material (ESI) for RSC Advances.

Supplemental Material

Human Bone Probed by Neutron Diffraction: the Burning Process

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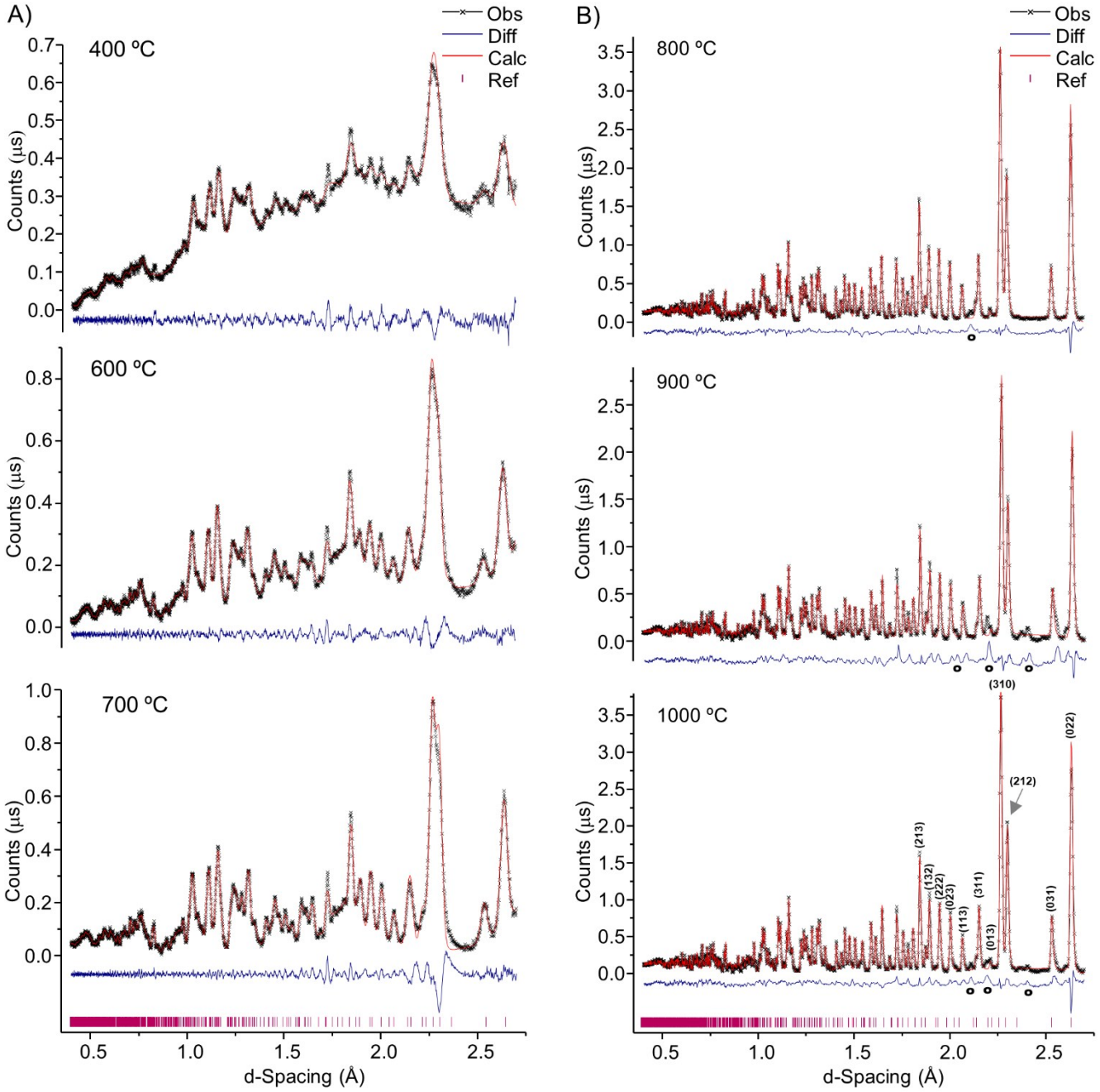

Figure S1.1 – Refined neutron diffraction data (Hist#5) for human femur (F41): (A) burned at 400, 600 and 700 ºC, using the Le Bail method and reference HAp (from NIST); (B) burned at 800, 900 and 1000 ºC, using the Rietveld method. (º Peaks different from those assigned to HAp).

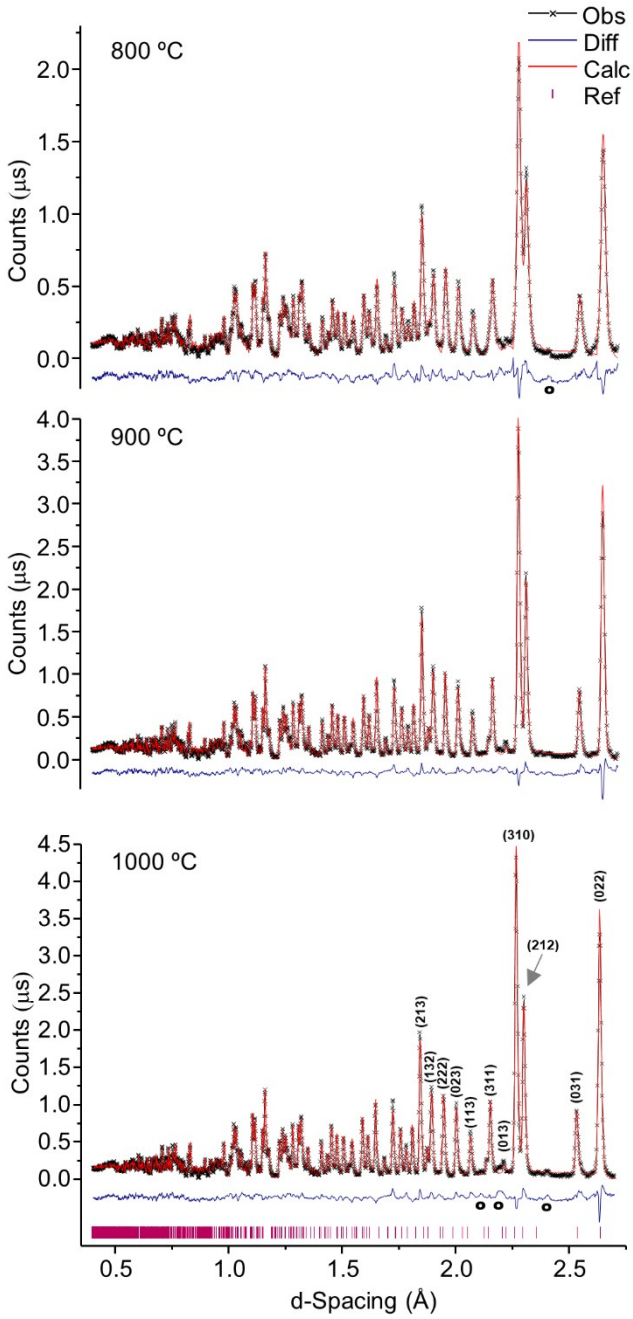

Figure S1.2 – Rietveld refined neutron diffraction data (Hist#5) for human humerus (H42) burned at 800, 900 and 1000 ºC, using reference HAp (from NIST) as a model. (º Peaks different from those assigned to HAp).

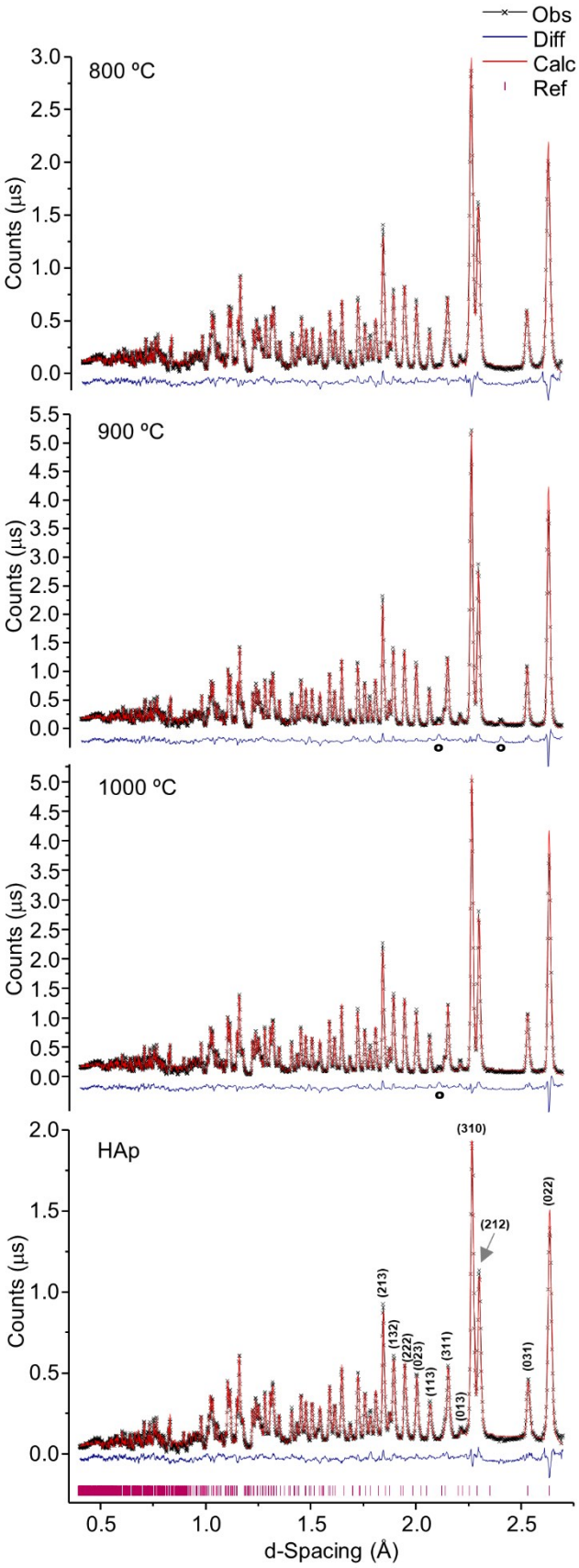

Figure S1.3 – Rietveld refined neutron diffraction data (Hist #5) for human femur (F42) burned at 800, 900 and 1000 ºC, using reference HAp (from NIST) as a model (which is also shown for comparison). (º Peaks different from those assigned to HAp).

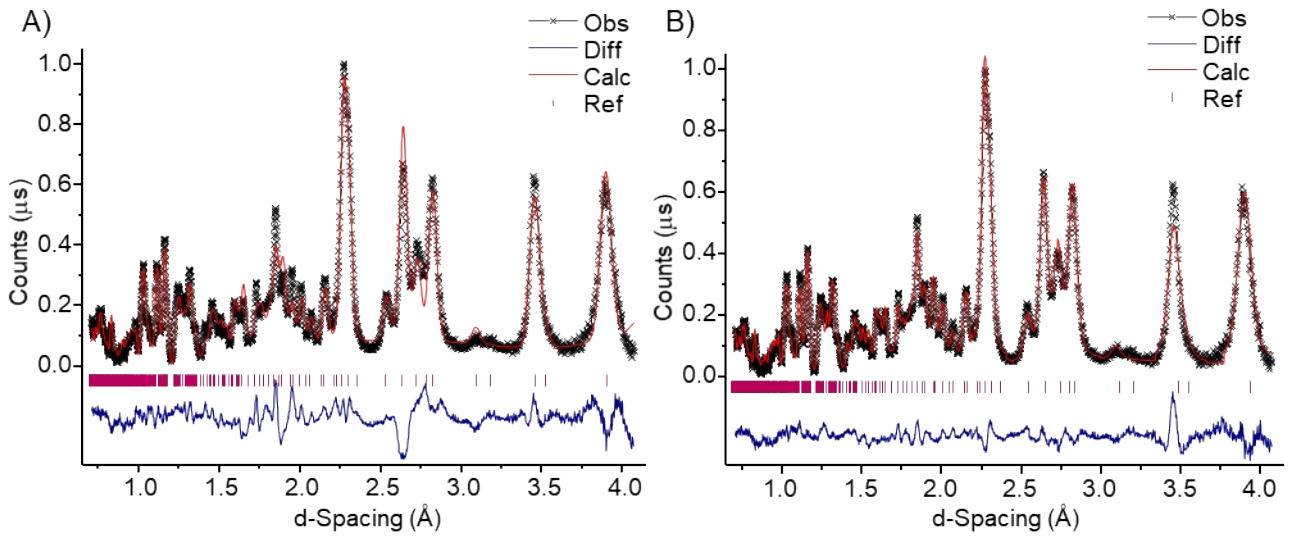

Figure S1.4 – Rietveld refined neutron diffraction data (Hist#4) for human femur (F42) burned at 700 ºC, using as a reference: (A) The carbonated apatite (BioHAp) model[1]; (B) The hydroxyapatite model[2].

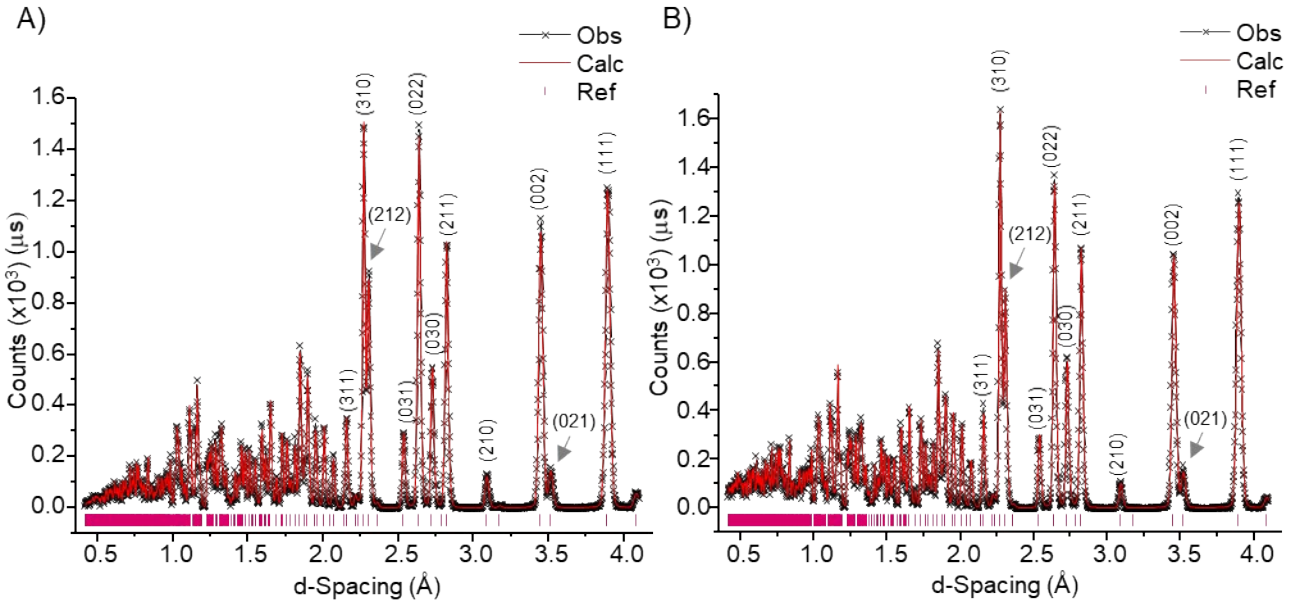

Figure S1.5 – Pattern simulation of the two reference models applied in the present study for GEM (Hist#4): (A) Carbonated apatite – BioHAp[1]; (B) Hydroxyapatite – Hap[2].

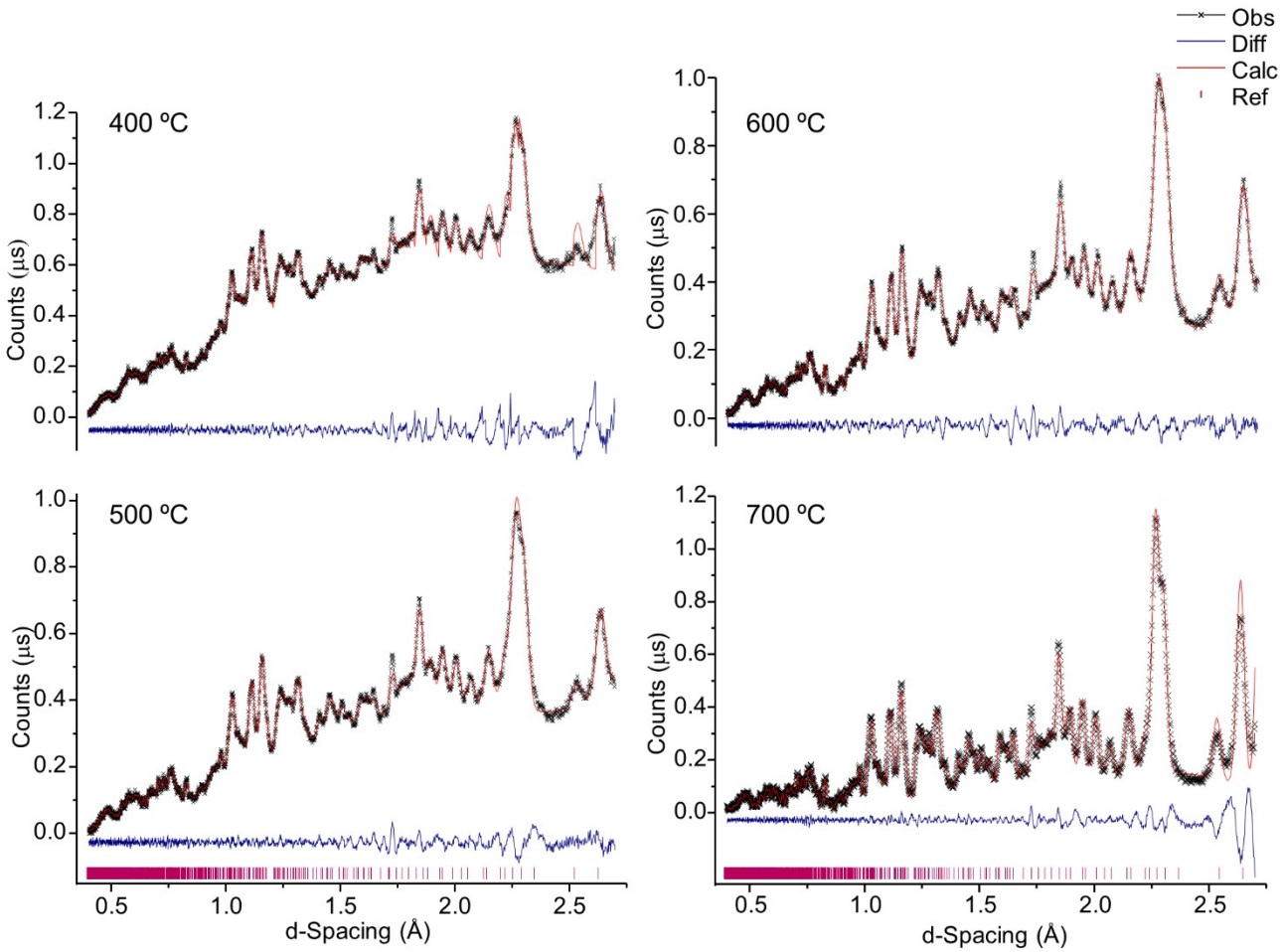

Figure S1.6 – Le Bail refined neutron diffraction data (Hist#5) for human femur (F42) burned at 400, 500, 600 and 700 ºC, using reference HAp (from NIST) as a model.

Figures S2 – FTIR-ATR

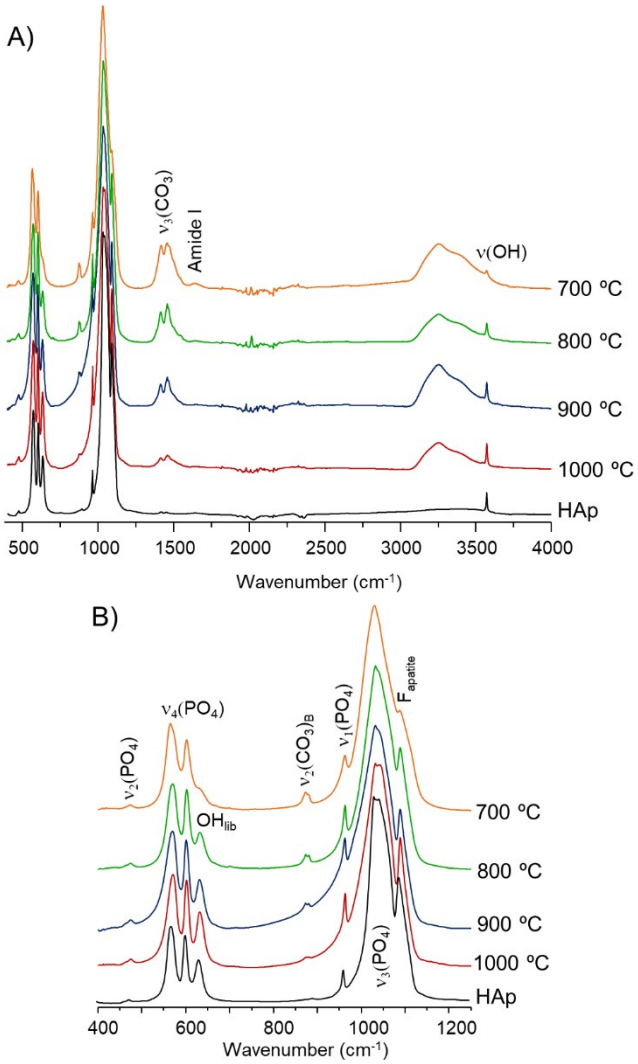

Figure S2.1 – FTIR-ATR spectra of human femur (F42) burned from 700 to 1000 ºC. (A) 400 – 4000 cm^{-1}; (B) 400 – 1250 cm^{-1}. (Reference hydroxyapatite is also shown for comparison. $F_{apatite}$ refers to fluorapatite).

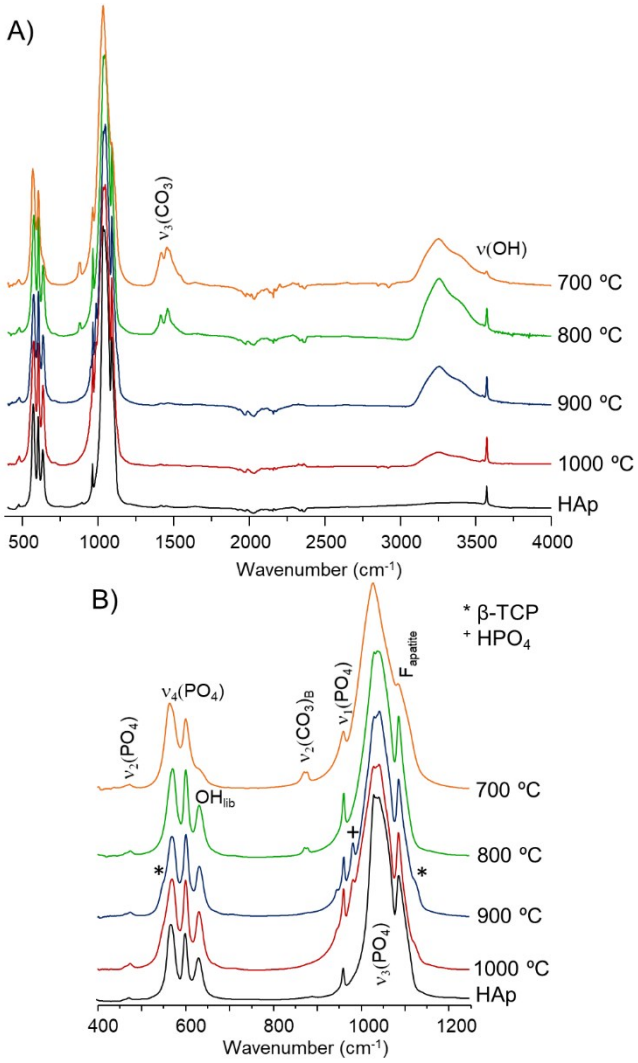

Figure S2.2 – FTIR-ATR spectra of human femur (F41) burned from 700 to 1000 ºC. (A) 400 – 4000 cm^{-1}; (B) 400 – 1250 cm^{-1}. (Reference hydroxyapatite is also shown for comparison. $F_{apatite}$ refers to fluorapatite).

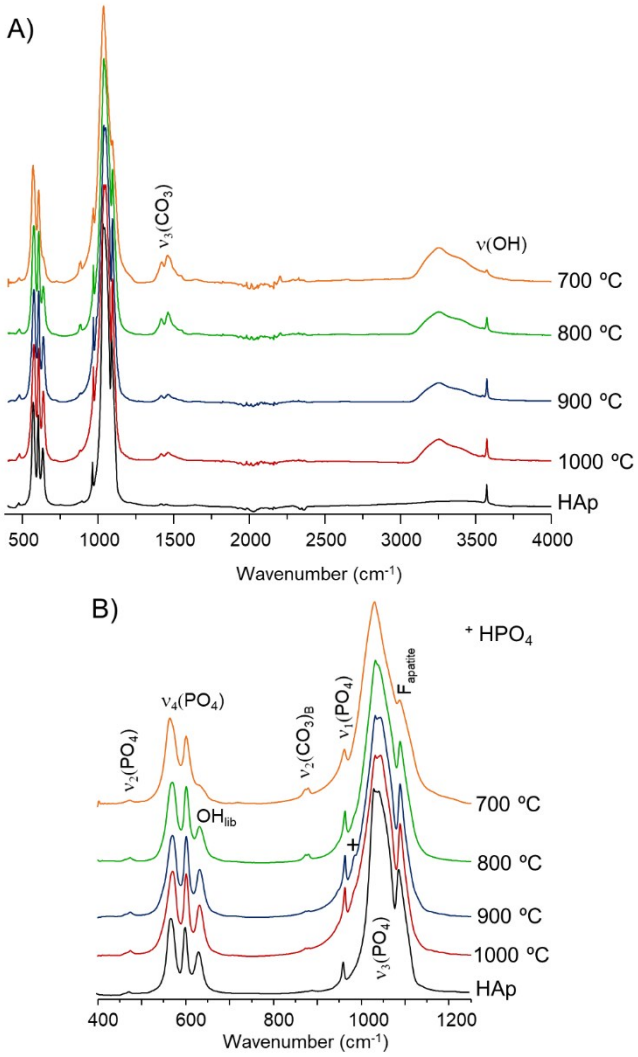

Figure S2.3 – FTIR-ATR spectra of human humerus (H42) burned from 700 to 1000 ºC. (A) 400 – 4000 cm^{-1}; (B) 400 – 1250 cm^{-1}. (Reference hydroxyapatite is also shown for comparison. $F_{apatite}$ refers to fluorapatite).

Table S1. Sig-1, Gam-2 and domain size values obtained after refinement for the samples under study and the respective error values.

Sample	Sig-1				Gam-2				p (Å)			
	Hist#5	*esd*	Hist#6	*esd*	Hist#5	*esd*	Hist#6	*esd*	Hist#5	*esd*	Hist#6	*esd*
HAp (NIST ref.)	8.7601E+01	3.6930	7.6836E+01	5.5010	6.80014	0.0806	7.60162	0.1874	981.694	1.207E-05	1194.776	2.063E-05
F41_1000ºC	1.3054E+02	3.3970	7.0841E+02	2.2980	2.33319	0.0688	1.81694	0.1449	2861.173	1.031E-05	4998.641	1.595E-05
F41_900ºC	1.1687E+02	4.9380	8.7852E+01	6.6790	3.94864	0.1058	4.24402	0.2290	1690.623	1.585E-05	2140.006	2.521E-05
F41_800ºC	1.1290E+02	2.8650	8.4390E+01	3.7510	3.98654	0.0636	3.85507	0.1353	1674.550	9.520E-06	2355.918	1.490E-05
F41_700ºC	1.6860E+03	11.4100	1.5850E+03	25.3800	34.3565	0.1606	43.8709	0.4648	194.306	2.406E-05	207.022	5.118E-05
F41_600ºC	2.2790E+03	23.3400	2.6090E+03	55.1900	37.9553	0.2989	52.0572	0.8950	175.882	4.477E-05	174.466	9.854E-05
F41_400ºC	4.4450E+03	59.6000	3.1710E+03	108.6000	44.7679	0.4965	56.9131	1.4460	149.117	7.437E-05	159.581	1.592E-04
F42_1000ºC	1.2814E+02	2.5130	9.5480E+01	3.3050	2.52304	0.0559	2.31848	0.1211	2645.880	8.371E-06	3917.321	1.333E-05
F42_900ºC	1.3270E+02	2.6920	9.8973E+01	3.6190	2.6703	0.0592	2.78678	0.1288	2499.966	8.867E-06	3259.041	1.418E-05
F42_800ºC	8.0340E+01	4.0490	7.6171E+01	6.2590	8.57663	0.0859	10.4996	0.1948	778.355	1.287E-05	865.007	2.145E-05
F42_700ºC	1.6507E+03	9.6240	2.2851E+03	26.9900	33.1184	0.1611	43.1778	0.4504	201.570	2.413E-05	210.345	4.959E-05
F42_600ºC	2.8450E+03	32.0800	3.3250E+03	80.3300	44.8149	0.3388	56.6747	0.9483	148.961	5.075E-05	160.252	1.044E-04
F42_500ºC	2.5480E+03	30.9600	2.7930E+03	73.2700	46.6957	0.3715	61.816	1.1980	142.961	5.565E-05	146.924	1.319E-04
F42_400ºC	2.7680E+03	36.1800	1.4400E+03	52.0400	34.4595	0.4113	43.9237	1.0640	193.725	6.161E-05	206.773	1.172E-04
H42_1000ºC	1.3252E+02	2.9970	9.4639E+01	3.8520	2.55008	0.0651	2.27605	0.1407	2617.824	9.747E-06	3990.347	1.549E-05
H42_900ºC	1.2355E+02	2.8570	9.2016E+01	3.7580	3.18845	0.0627	3.1092	0.1357	2093.701	9.388E-06	2921.083	1.494E-05
H42_800ºC	3.7348E+01	6.3710	6.9300E+02	8.9350	13.9264	0.1320	18.554	0.3233	479.353	1.977E-05	489.503	3.560E-05
T42_1000ºC	1.3186E+02	5.2730	9.6709E+01	7.2660	2.62072	0.1127	2.89558	0.2554	2547.262	1.688E-05	3136.584	2.812E-05
T42_900ºC	1.1125E+02	3.2100	8.4214E+01	4.3350	3.46563	0.0715	3.30509	0.1605	1926.247	1.071E-05	2747.952	1.767E-05
T42_800ºC	2.9550E+01	10.3900	6.4430E+01	24.5300	19.5742	0.1892	29.0205	0.5057	341.044	2.834E-05	312.959	5.568E-05
T42_700ºC	1.4830E+03	10.3900	1.3500E+03	21.9400	31.5338	0.1576	39.9399	0.4523	211.699	2.361E-05	227.397	4.980E-05
T42_600ºC	1.7610E+03	17.3600	2.0060E+03	43.6400	32.4704	0.2427	42.9841	0.7398	205.592	3.636E-05	211.293	8.146E-05
T42_400ºC	2.5490E+03	37.1600	2.9190E+03	77.2100	107.345	1.2450	104.058	2.4130	62.189	1.865E-04	87.280	2.657E-04

Figure S3

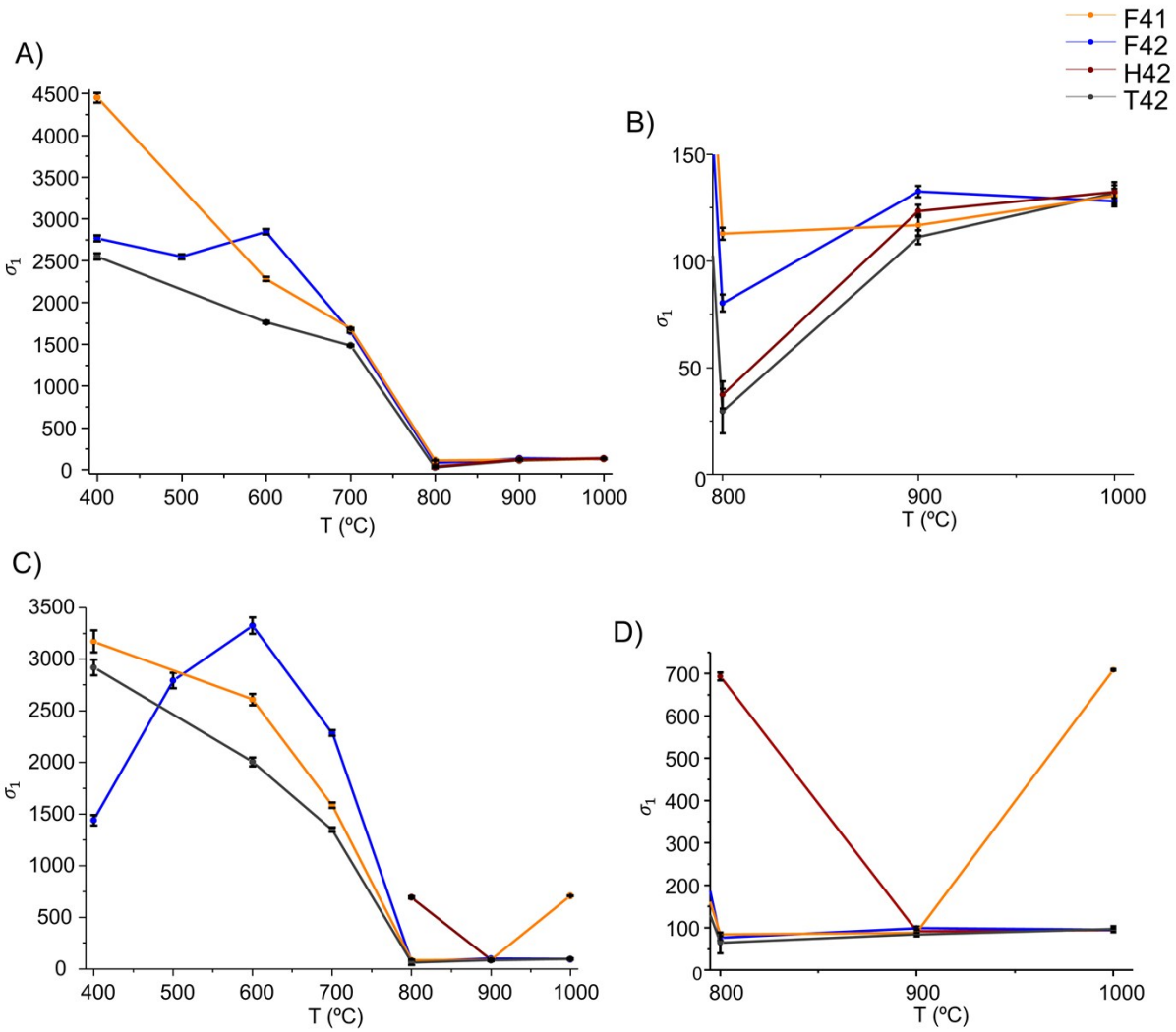

Figure S3 – Graphical representation of parameter Sig-1: (A) for Hist#5 as a function of temperature; (B) for Hist#5 in the 800-1000ºC range; (C) for Hist#6 as a function of temperature and (D) for Hist#6 in the 800-1000ºC range.

References:

1. M. E. Fleet, X. Y. Liu and P. L. King, *American Mineralogist*, 2004, **89**, 1422-1432.
2. M. I. Kay, R. A. Young and A. S. Posner, *Nature*, 1964, **204**, 1050-2.