

## Supplementary Material

# Partners in Postmortem Interval Estimation: X-ray Diffraction and Fourier Transform Spectroscopy

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**Table S1.** Correlation matrix among crystallographic indexes and compositional parameters in human teeth.

Variables	Age	Crystallinity	Crystal size	M/M ratio	C/P ratio	Mineral maturity	Collagen maturity
PMI	0.407 <b>0.009</b>	0.500 <b>0.001</b>	0.363 <b>0.021</b>	0.732 <b>&lt;0.001</b>	-0.328 <b>0.039</b>	-0.190 ns	-0.194 ns
Crystallinity			0.360 <b>0.022</b>	0.426 <b>0.006</b>	-0.505 <b>0.001</b>	0.117 ns	-0.159 ns
Crystal size				0.257 ns	-0.236 ns	0.112 ns	-0.076 ns
M/M ratio					-0.654 <b>&lt;0.001</b>	-0.099 ns	-0.145 ns
C/P ratio						0.040 ns	-0.033 ns
Mineral maturity							0.232 ns

Collagen maturity
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Correlation matrix showing correlation coefficients between a single variable and every other variable. *p*-values are also shown (significance in bold).

**Table S2.** Correlation matrix among crystallographic indexes and compositional parameters in human male teeth.

Variables	Age	Crystallinity	Crystal size	M/M ratio	C/P ratio	Mineral maturity	Collagen maturity
PMI	0.615 <b>0.004</b>	0.382 ns	0.241 ns	0.641 <b>0.002</b>	-0.020 ns	-0.324 ns	-0.401 ns
Crystallinity			0.362 ns	0.189 ns	-0.333 ns	-0.016 ns	-0.373 ns
Crystal size				0.049 ns	-0.021 ns	0.401 ns	-0.030 ns
M/M ratio					-0.492 <b>0.028</b>	-0.449 <b>0.047</b>	-0.295 ns
C/P ratio						0.257 ns	-0.020 ns
Mineral maturity							0.277 ns
Collagen maturity							

Correlation matrix showing correlation coefficients between a single variable and every other variable. *p*-values are also shown (significance in bold).

**Table S3.** Correlation matrix among crystallographic indexes and compositional parameters in human female teeth.

Variables	Age	Crystallinity	Crystal size	M/M ratio	C/P ratio	Mineral maturity	Collagen maturity
PMI	0.302 ns	0.601 <b>0.005</b>	0.475 <b>0.034</b>	0.837 <b>&lt;0.001</b>	-0.763 <b>&lt;0.001</b>	-0.093 ns	-0.029 ns
Crystallinity			0.392 ns	0.651 <b>0.002</b>	-0.757 <b>&lt;0.001</b>	0.199 ns	-0.021 ns
Crystal size				0.406 ns	-0.363 ns	-0.018 ns	-0.097 ns
M/M ratio					-0.909 <b>&lt;0.001</b>	0.186 ns	-0.005 ns
C/P ratio						-0.168 ns	-0.091 ns
Mineral maturity							0.207 ns

Collagen maturity

Correlation matrix showing correlation coefficients between a single variable and every other variable. *p*-values are also shown (significance in bold).

**Table S4.** Crystallographic indexes and compositional parameters with high loadings in extracted components that contribute towards PMI (0-10-25-50 years) in human teeth.

Variables	Component 1 (34.1%)	Component 2 (19.8%)	Component 3 (16.7%)
M/M ratio	0.875	-	-
C/P ratio	-0.789	-	-
Age	0.666	-0.401	-
Crystallinity	0.578	0.557	-
Crystal size	-	0.840	-
Mineral maturity	-	-	0.797
Collagen maturity	-	-	0.735

Rotated orthogonal (varimax) component matrix from principal component analysis. A factor loading >0.4 was considered high enough for interpretation (shown). Components together explain 70.5% of the variance that contribute towards PMI.  $\chi^2 = 34.64$ ,  $p < 0.001$ .

**Table S5.** Crystallographic indexes and compositional parameters as predictors for PMI in human teeth.

Variables	0-10 PMI			0-25 PMI			0-50 PMI		
	B	Wald $\chi^2$	<i>p</i>	B	Wald $\chi^2$	<i>p</i>	B	Wald $\chi^2$	<i>p</i>
(Intercept)	133.908	1.393	0.238	-41.077	2.840	0.092	-20.919	4.077	<b>0.043</b>
Crystallinity	0.569	2.420	0.120	0.817	3.893	<b>0.048</b>	0.457	5.735	0.017
Crystal size	1.403	3.191	0.074	-	-	-	-	-	-
M/M ratio	-14.862	2.604	0.107	-	-	-	-	-	-
C/P ratio	-811.79	2.084	0.149	-	-	-	-	-	-
Mineral maturity	-	-	-	-10.658	2.865	0.091	-7.901	2.834	0.092
Collagen maturity	-	-	-	-	-	-	-	-	-
Age	-	-	-	-	-	-	-	-	-
Backward step	3			6			6		
Cox & Snell $R^2$		0.604			0.508			0.445	
Nagelkerke $R^2$		0.806			0.677			0.593	
Sensitivity		0.9			0.9			0.9	
1-Specificity		0.1			0.2			0.2	

95% CI	0.875-1.045	0.755-1.044	0.803-1.037
AUC	0.96	0.90	0.92
Overall rate	87%	76%	80%

Logistic regression (backward method). Variables entered on step 1: age, crystallinity, crystal size, mineral-to-matrix (M/M) ratio, carbonate substitution (C/P ratio), mineral maturity and collagen maturity. A stepping method criteria of 0.05 (entry), 0.2 (removal) and 0.5 (cutoff) were considered. *p*-values are also shown (significance in bold).

**Table S6.** Characteristics of the samples.

SEX	AGE	TEETH*	PMI (years)
Male	55	28	0
Female	59	44	0
Male	50	44	0
Male	57	27	0
Female	77	45	0
Male	60	38	0
Male	50	25	0
Female	74	44	0
Female	57	38	0
Female	80	44	0
Male	51	37	10
Female	53	28	10

Male	55	28	10
Female	40	36	10
Male	39	38	10
Female	53	25	10
Female	42	44	10
Male	51	14	10
Female	29	28	10
Male	74	25	10
Male	58	25	25
Female	59	24	25
Male	60	45	25
Male	62	45	25
Female	56	45	25
Female	64	14	25
Male	56	45	25
Male	65	25	25
Female	63	34	25
Female	60	44	25
Male	68	17	50
Female	62	27	50
Female	82	45	50
Male	68	44	50
Male	73	44	50
Female	68	44	50
Female	82	34	50
Male	65	35	50
Male	61	35	50
Female	62	27	50

\*Teeth are listed according to the FDI nomenclature . PMI: Postmortem Interval