

## Supplementary Materials

### Influence of phase composition and morphology on the calcium ion release of several classical and hybrid endodontic cements

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Table S1. Phase composition according to XRD analyses

Cement	Main phase	Main phase	Main phase	Main phase	Radiopacifier	Trace phases
<b>TheraCal LC</b>	Ca <sub>3</sub> SiO <sub>5</sub> ICDD-PDF2#00-049-0442 (Main peaks at 2θ - 29.23, 32.06, 32.38)		Ca <sub>3</sub> Al <sub>2</sub> O <sub>6</sub> ICDD-PDF2#00-038-1429 (Main peaks at 2θ - 33.09, 47.33, 59.24)	Ca <sub>2</sub> SiO <sub>4</sub> ICDD-PDF2#00-061-0379 (Main peaks at 2θ - 25.71, 31.80, 33.02)	Ba <sub>2</sub> CaWO <sub>6</sub> ICDD-PDF2#01-073-0136 (Main peaks at 2θ - 30.08, 43.11, 53.34)	
<b>Soaked TheraCal LC</b>	Ca <sub>3</sub> SiO <sub>5</sub> ICDD-PDF2#00-049-0442 (Main peaks at 2θ - 29.23, 32.06, 32.38)	C-CaCO <sub>3</sub> ICDD-PDF2#00-024-0027 (Main peaks at 2θ - 22.94, 29.49, 39.43)	Ca <sub>3</sub> Al <sub>2</sub> O <sub>6</sub> ICDD-PDF2#00-038-1429 (Main peaks at 2θ - 33.09, 47.33, 59.24)		Ba <sub>2</sub> CaWO <sub>6</sub> ICDD-PDF2#01-073-0136 (Main peaks at 2θ - 30.08, 43.11, 53.34)	Ca-Al-Si-O ICDD-PDF2#00-014-0081
<b>BioCal® Cap</b>	Ca <sub>3</sub> SiO <sub>5</sub> ICDD-PDF2#00-049-0442 (Main peaks at 2θ - 29.23, 32.06, 32.38)		Ca <sub>3</sub> Al <sub>2</sub> O <sub>6</sub> ICDD-PDF2#00-038-1429 (Main peaks at 2θ - 33.09, 47.33, 59.24)	Ca <sub>2</sub> SiO <sub>4</sub> ICDD-PDF2#00-061-0379 (Main peaks at 2θ - 25.71, 31.80, 33.02)	BaSO <sub>4</sub> ICDD-PDF2#01-070-7037 (Main peaks at 2θ - 25.80, 26.96, 28.80)	
<b>Soaked BioCal® Cap</b>	Ca <sub>3</sub> SiO <sub>5</sub>			Ca <sub>2</sub> SiO <sub>4</sub>	BaSO <sub>4</sub>	

	ICDD-PDF2#00-049-0442 (Main peaks at 2θ - 29.23, 32.06, 32.38)		ICDD-PDF2#00-061-0379 (Main peaks at 2θ - 25.71, 31.80, 33.02)	ICDD-PDF2#01-070-7037 (Main peaks at 2θ - 25.80, 26.96, 28.80)
<b>Harvard MTA Universal initial powder mixture</b>	Ca <sub>3</sub> SiO <sub>5</sub> ICDD-PDF2#00-049-0442 (Main peaks at 2θ - 29.23, 32.06, 32.38)		Ca <sub>2</sub> SiO <sub>4</sub> ICDD-PDF2#00-061-0379 (Main peaks at 2θ - 25.71, 31.80, 33.02)	CaWO <sub>4</sub> ICDD-PDF2#01-071-6152 (Main peaks at 2θ - 18.64, 28.77, 31.40)
<b>Harvard MTA Universal solidified mixture</b>	Ca <sub>3</sub> SiO <sub>5</sub> ICDD-PDF2#00-049-0442 (Main peaks at 2θ - 29.23, 32.06, 32.38)	C-CaCO <sub>3</sub> ICDD-PDF2#00-024-0027 (Main peaks at 2θ - 22.94, 29.49, 39.43)	Ca <sub>3</sub> Al <sub>2</sub> O <sub>6</sub> ICDD-PDF2#00-038-1429 (Main peaks at 2θ - 33.09, 47.33, 59.24)	CaWO <sub>4</sub> ICDD-PDF2#01-071-6152 (Main peaks at 2θ - 18.64, 28.77, 31.40)
<b>Soaked Harvard MTA Universal</b>		C-CaCO <sub>3</sub> ICDD-PDF2#00-024-0027 (Main peaks at 2θ - 22.94, 29.49, 39.43) V-CaCO <sub>3</sub> ICDD-PDF2#00-024-0030 (Main peaks at 2θ - 24.91, 27.04, 32.66)		CaWO <sub>4</sub> ICDD-PDF2#01-071-6152 (Main peaks at 2θ - 18.64, 28.77, 31.40) Ca-Al-Si-O ICDD-PDF2#00-014-0081 Ca <sub>2</sub> Al <sub>3</sub> Si <sub>3</sub> O <sub>12</sub> (OH)
<b>Rootdent initial powder mixture</b>	Ca <sub>3</sub> SiO <sub>5</sub> ICDD-PDF2#00-049-0442 (Main peaks at 2θ - 29.23, 32.06, 32.38)			ZrO <sub>2</sub> ICDD-PDF2#00-024-1165 (Main peaks at 2θ - 24.01, 28.22, 31.45)
<b>Rootdent</b>	Ca <sub>3</sub> SiO <sub>5</sub>			ZrO <sub>2</sub> amorphous

<b>solidified mixture</b>	ICDD-PDF2#00-049-0442 (Main peaks at 2θ - 29.23, 32.06, 32.38)			ICDD-PDF2#00-024-1165 (Main peaks at 2θ - 24.01, 28.22, 31.45)	
<b>Soaked Rootdent</b>	Ca <sub>3</sub> SiO <sub>5</sub> ICDD-PDF2#00-049-0442 (Main peaks at 2θ - 29.23, 32.06, 32.38)	A-CaCO <sub>3</sub> ICDD-PDF2#00-001-0628 (Main peaks at 2θ - 26.16, 33.15, 45.82)		ZrO <sub>2</sub> ICDD-PDF2#00-024-1165 (Main peaks at 2θ - 24.01, 28.22, 31.45)	Ca-Al-Si-O ICDD-PDF2#00-014-0081 Ca <sub>2</sub> Al <sub>2</sub> SiO <sub>7</sub> ·8H <sub>2</sub> O Ca <sub>4</sub> Al <sub>2</sub> O <sub>6</sub> (CO <sub>3</sub> ) <sub>0.5</sub> (OH)·11.5 H <sub>2</sub> O Ca <sub>4</sub> Al <sub>2</sub> O <sub>6</sub> CO <sub>3</sub> ·11H <sub>2</sub> O
<b>BioFactor</b>	Ca <sub>3</sub> SiO <sub>5</sub> ICDD-PDF2#00-049-0442 (Main peaks at 2θ - 29.23, 32.06, 32.38)	Ca <sub>3</sub> Al <sub>2</sub> O <sub>6</sub> ICDD-PDF2#00-038-1429 (Main peaks at 2θ - 33.09, 47.33, 59.24)	Ca <sub>2</sub> SiO <sub>4</sub> ICDD-PDF2#00-061-0379 (Main peaks at 2θ - 25.71, 31.80, 33.02)	Yb <sub>2</sub> O <sub>3</sub> ICDD-PDF2#01-072-8494 (Main peaks at 2θ - 29.66, 34.36, 49.37)	
<b>Soaked BioFactor</b>		V-CaCO <sub>3</sub> ICDD-PDF2#00-024-0030 (Main peaks at 2θ - 24.91, 27.04, 32.66) A-CaCO <sub>3</sub> ICDD-PDF2#00-001-0628 (Main peaks at 2θ - 26.16, 33.15, 45.82) C-CaCO <sub>3</sub> ICDD-PDF2#00-024-0027 (Main peaks at 2θ - 22.94, 29.49, 39.43)		Yb <sub>2</sub> O <sub>3</sub> ICDD-PDF2#01-072-8494 (Main peaks at 2θ - 29.66, 34.36, 49.37)	Ca-Al-Si-O ICDD-PDF2#00-014-0081

<b>BioFactor (PDT)</b>	Ca <sub>3</sub> SiO <sub>5</sub> ICDD-PDF2#00- 049-0442 (Main peaks at 2θ - 29.23, 32.06, 32.38)	Yb <sub>2</sub> O <sub>3</sub> ICDD-PDF2#01- 072-8494 (Main peaks at 2θ - 29.66, 34.36, 49.37)
<b>Soaked BioFactor (PDT)</b>	V-CaCO <sub>3</sub> ICDD-PDF2#00-024- 0030 (Main peaks at 2θ - 24.91, 27.04, 32.66) C-CaCO <sub>3</sub> ICDD-PDF2#00-024- 0027 (Main peaks at 2θ - 22.94, 29.49, 39.43)	Yb <sub>2</sub> O <sub>3</sub> ICDD-PDF2#01- 072-8494 (Main peaks at 2θ - 29.66, 34.36, 49.37)
		Ca-Al-Si-O ICDD-PDF2#00- 014-0081