Supplementary

Calcium Chelidonate: Semi-synthesis, Crystallography, and Osteoinductive Activity In Vitro and In Vivo

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Table S1. Crystallographic parameters and details of experiment solution and refinement for semi-synthetic (**II**) and natural (**I**) forms of $[Ca(ChA)(H_2O)_3]_n$

	avd2_synt (**II**)	avd2_nat (**I**)
Empirical formula	$C_7H_8CaO_9$	$C_7H_8CaO_9$
Formula weight	276.21	276.21
Crystal system	Orthorhombic	Orthorhombic
Space group	Pna2(1)	Pna2(1)
Unit cell dimensions	a = 8.380(2) A alpha = 90 deg.	a = 8.419(13) A alpha = 90 deg.
	b = 19.702(4) A beta = 90 deg	b = 19.82(3) A beta = 90 deg.
	c = 6.1653(14) A gamma = 90 de	c = 6.207(8) A gamma = 90 deg.
Volume	1017.9(4) A^3	1036(3) A^3
Z, Calculated density	4, 1.802 Mg/m^3	4, 1.772 Mg/m^3
Absorption coefficient	0.655 mm^{-1}	0.644 mm^{-1}
F(000)	568	568
Crystal size	0.30 x 0.09 x 0.005 mm	0.30 x 0.09 x 0.01 mm
Theta range for data collection	2.64 to 25.93 deg.	2.63 to 24.79 deg.

Limiting indices	-9<=h<=10, -24<=k<=24, -7<=l<=7	-8<=h<=9, -23<=k<=20, -7<=l<=6
Reflections collected / unique	9349 / 1966 [R(int) = 0.0487]	4896 / 1608 [R(int) = 0.1379]
Completeness to theta = 24.79	99.1 %	99.1 %
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents
Max. and min. transmission	0.8620 and 0.7714	0.8620 and 0.5294
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	1966 / 7 / 179	1608 / 11 / 166
Goodness-of-fit on F^2	1.065	1.000
Final R indices [I>2sigma(I)]	R1 = 0.0347, wR2 = 0.0765	R1 = 0.0721, wR2 = 0.1508
R indices (all data)	R1 = 0.0446, wR2 = 0.0801	R1 = 0.1230, wR2 = 0.1716
Absolute structure parameter	0.12(4)	0.00(12)
Largest diff. peak and hole	0.322 and -0.220 $e.A^{-3}$	0.716 and -0.603 $e.A^{-3}$