

Oligomer formation, metalation, and the existence of  
aggregation-prone and mobile sequences within the  
intracrystalline protein family, Asprich. Electronic Supporting  
Information.

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Table S1: ESI-MS ion trap Asprich “3” protein – cation adduct species.

Sample	Peak (Fig 2)	Adduct Species	Observed Peak (m/z)	Theoretical (m/z)
Apo Asprich “3”		$[M - 12H^+]^{12-}$	551.3	551.3
		$[M - 11H^+]^{11-}$	601.3	601.4
		$[M - 10H^+]^{10-}$	661.3	661.7
		$[M - 9H^+]^{9-}$	734.9	735.3
		$[M - 8H^+]^{8-}$	826.9	827.4
		$[M - 7H^+]^{7-}$	945.2	945.7
		$[M - 6H^+]^{6-}$	1102.8	1103.5
Asprich “3”-Eu <sup>3+</sup>		$[M + Eu^{3+} - 10H^+]^{7-}$	754.1	754.3
	a	$[M + Eu^{3+} - 13H^+]^{10-}$	810.2	810.6
	b	$[M + Eu^{3+} - 19H^+]^{16-}$	868.0	868.0
		$[M + Eu^{3+} - 9H^+]^{6-}$	886.0	887.2
		$[M + Eu^{3+} - 33H^+]^{30-}$	946.0	946.3
		$[M + Eu^{3+} - 54H^+]^{51-}$	925.0	925.1
		$[M + 3Eu^{3+} - 12H^+]^{3-}$	1007.0	1007.0
		$[M + 2Eu^{3+} - 25H^+]^{19-}$	1013.0	1013.1
		$[M + Eu^{3+} - 30H^+]^{27-}$	1067.1	1067.6
	Asprich “3” - La <sup>3+</sup>		$[M + La^{3+} - 30H^+]^{27-}$	770.0
A		$[M + 2La^{3+} - 51H^+]^{45-}$	827.9	828.0
B		$[M + 2La^{3+} - 33H^+]^{27-}$	845.9	846.0
		$[M + 3La^{3+} - 14H^+]^{5-}$	1015.7	1015.1
Asprich “3” -Ca <sup>2+</sup>		$[M + Ca^{2+} - 12H^+]^{10-}$	590.0	590.3
		$[M + 3Ca^{2+} - 23H^+]^{17-}$	648.0	648.3
		$[M + Ca^{2+} - 11H^+]^{9-}$	700.0	700.5
		$[M + 4Ca^{2+} - 14H^+]^{6-}$	758.0	758.4
	1	$[M + 2Ca^{2+} - 12H^+]^{8-}$	811.9	811.9
	2	$[M + 4Ca^{2+} - 12H^+]^{4-}$	819.9	820.5
	3	$[M + 4Ca^{2+} - 25H^+]^{17-}$	869.8	869.9
		$[M + 3Ca^{2+} - 23H^+]^{17-}$	931.8	931.9
		$[M + 3Ca^{2+} - 10H^+]^{4-}$	945.2	945.4

Units of mass are in Daltons (Da). Peak identifiers (numeric or alphabetic) are given on Figure 2 over the assigned monoisotopic centroid peaks.