Electronic Supplementary Material (ESI) for CrystEngComm.

Supplementary information

Magnetic particles used in a new approach for designed protein crystallization

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The effect of magnetic particles as additives in crystallization

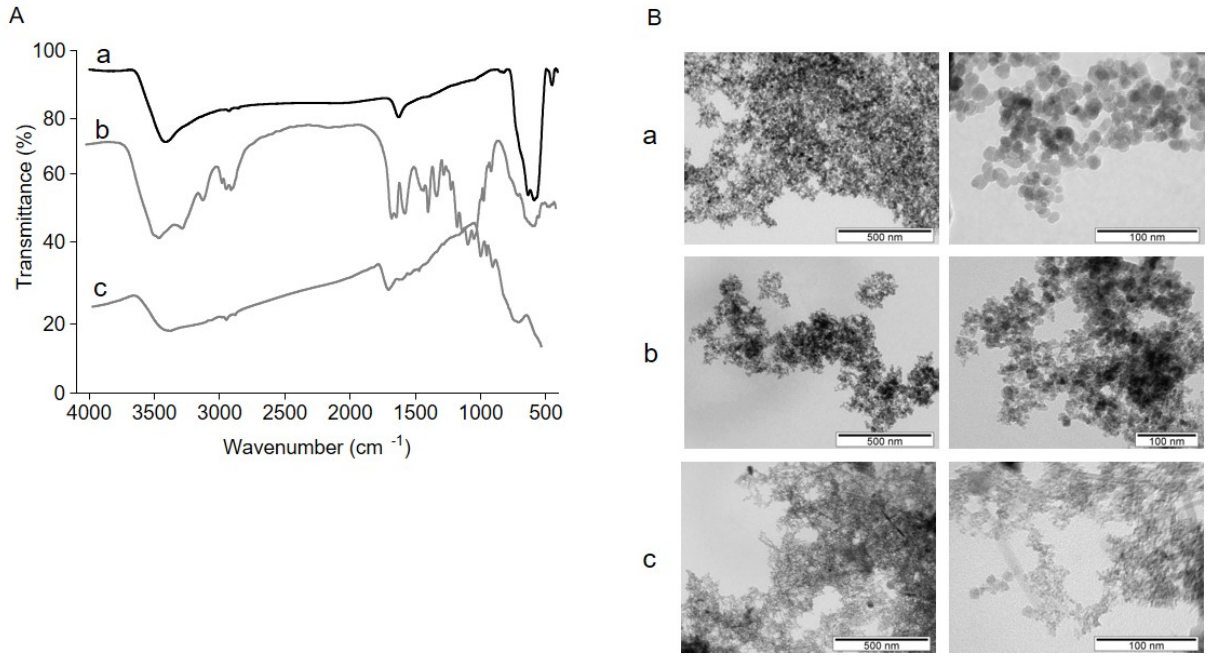

Figure SI 1. Characterization of iron oxide magnetic particles (1 mg/ml) by (A) FT-IR and (B) Transmission electron microscopy analysis. Legend: (a) MP-Fe_3O_4; (b) MP-chitin; (c) MP-casein.

Table SI 1. Characterization of iron oxide magnetic particles (1 mg/ml) characterization by DLS and zeta potential in different crystallization conditions

	MP / Condition	MP-Fe_3O_4	MP-chitin	MP-casein	MP-A4C7
DLS (nm)	Water	100.9 ± 0.1	245.5 ± 0.4	8243.5 ± 1579.6	6482.3 ± 784.9
	0.5 M NaCl	5134.8 ± 651.4	4102.0 ± 709.1	-	-
	3 mM $CaCl_2$ with benzamidine	95.99 ± 0.85	-	10665 ± 586	-
	3 mM $CaCl_2$	5446.7 ± 2050.8	-	10556.3 ± 1556.4	-
	20% (w/v) PEG8000	231.8 ± 14.3	-	-	1331.0 ± 187.7
Zeta potential (mV)	Water	-0.6 ± 0.4	-15.8 ± 0.4	-6.9 ± 1.8	-1.5 ± 0.6
	0.5 M NaCl	10.3 ± 2.8	-13.5 ± 2.2	-	-
	3 mM $CaCl_2$ with benzamidine	23.1 ± 2.8	-	9.7 ± 1.9	-
	3 mM $CaCl_2$	-0.4 ± 0.3	-	14.1 ± 0.5	-
	20% (w/v) PEG8000	-54.0 ± 1.9	-	-	-42.1 ± 3.6

The effect of affinity-triggered magnetic crystallization

Table SI 2. Affinity data for the fitting of the affinity pairs HEWL::Fe_3O_4 / HEWL::MP-chitin and trypsin::MP- Fe_3O_4 / trypsin::MP-casein in the presence and absence of benzamidine. The experimental results were fitted to the Hill plot $q = Q_{max} \times Ka \times C^{1-n}/(1 + Ka \times C^{1-n})$, where q is the bound protein per mass of support (mg/g support) and C corresponds to the concentration of unbound protein in equilibrium (mg/ml) (R^2 >0.9).

	HEWL		**Trypsin**			
	MP-Fe_3O_4	**MP-chitin**	**MP-Fe_3O_4**		**MP-casein**	
			Benzamidine	No benzamidine	Benzamidine	No benzamidine
Q_{max} (mg/g support)	16021.6 ± 24418.9	6311.7 ± 1328.1	999.6 ± 86.2	2221.1 ± 279.1	1283.6 ± 74.0	2709.5 ± 552.8
K_a (M^{-1})	1.2 x10^7	1.1 x10^7	7.9 x10^3	2.4 x10^4	4.4 x10^3	2.4 x10^4
n (Hill coefficient)	1.2 ± 0.4	1.4 ± 0.4	2.1 ± 0.7	2.5 ± 0.7	1.7 ± 0.4	1.7 ± 0.5

Selected diffraction images

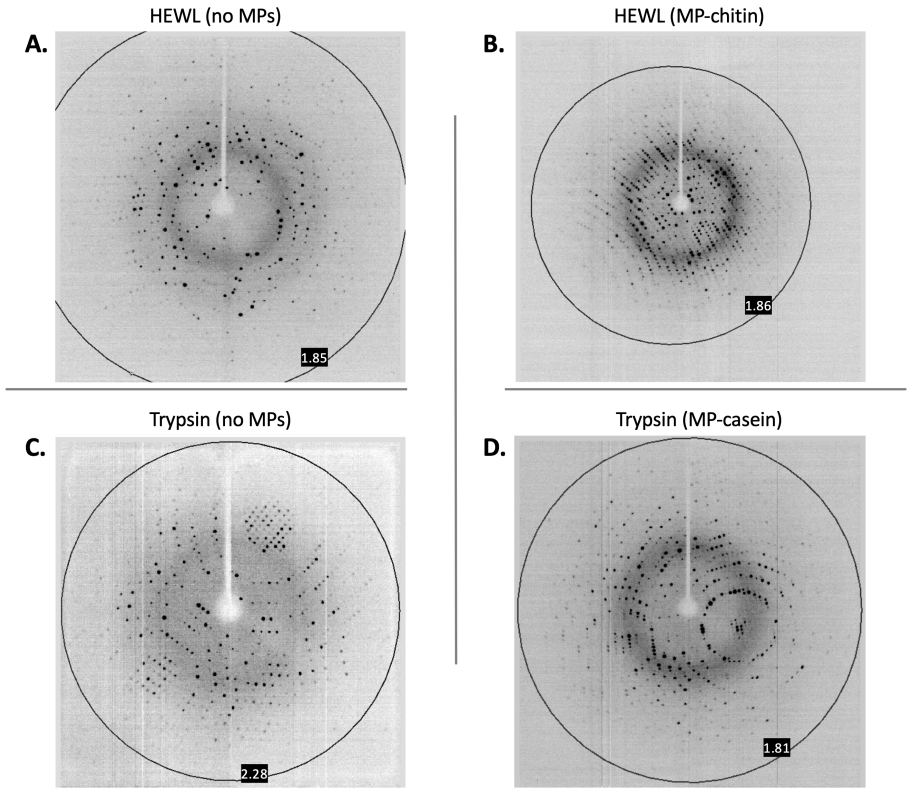

Figure SI 2. Selected X-ray diffraction images representative of the data collections carried out at the in-house X-ray diffraction facility using a Bruker D8 Venture Cu K_α diffractometer. **A.** Diffraction image of a HEWL single crystal grown in the absence of MPs. Exposure time: 10s; crystal-to-detector distance: 46.00mm; 2theta: -1.80°; ΔPhi: 0.50°. **B.** Diffraction image of a HEWL single crystal grown in the presence of MP-chitin. Exposure time: 10s; crystal-to-detector distance: 34.00mm; 2theta: -4.01°; ΔPhi: 0.50°. **C.** Diffraction image of a bovine pancreas trypsin single crystal grown in the absence of MPs. Exposure time: 30s; crystal-to-detector distance: 58.00mm; 2theta: 0.00°; ΔPhi: 0.50°. **D.** Diffraction image of a bovine pancreas trypsin single crystal grown in the presence of MP-casein. Exposure time: 10s; crystal-to-detector distance: 40.00mm; 2theta: 0.00°; ΔPhi: 0.50°. Approximate maximum resolution limits for each crystal are indicated by a black line circle (values in angstroms).