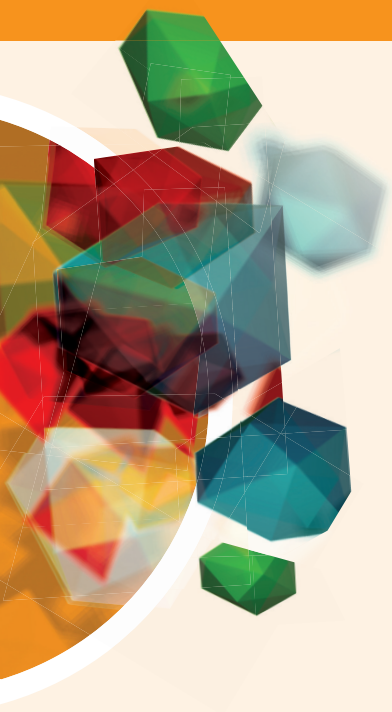
XP Screens
Crystal Screening with the Protein Crystal Glue TEW

Jena Bioscience
Building Blocks of Life



The **XP Screen** is a convenient initial screen that has successfully induced protein crystallization with low TEW concentrations such as 1 mM[5,6]. In some cases however, higher concentration of 5 or 10 mM TEW are needed.

The **XP Up Screen** is an upgrade of the well-established XP Screen. It contains 96 of the most prominent screening solutions that are long-term stable in the presence of up to 10 mM TEW.

Advantages of XP Screens

- Convenient initial screening with up to 10 mM TEW
- Improved crystal quality and resolution
- Tight crystal contacts
- New crystal forms (e.g to provide access to binding pockets)
- Direct phasing

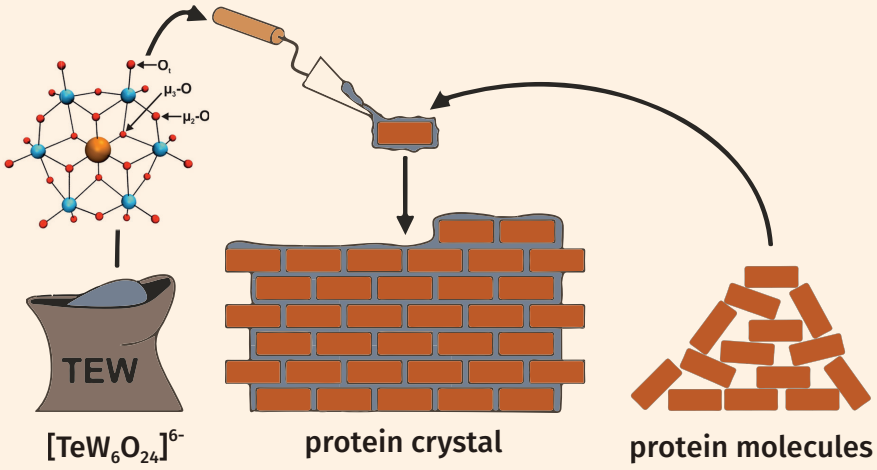


Figure from [1].

Product	Cat.-No.	Amount
XP Screen	CS-350	96 screening conditions with 1 mM TEW
XP Up Screen	CS-351	96 screening conditions to be upgraded with up to 10 mM TEW
Anderson-Evans polyoxotungstate (TEW)	X-TEW-5	Additive for optimization

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The Anderson-Evans Polyoxotungstate $[TeW_6O_{24}]^{6-}$ (TEW) is a universal and flexible crystallization additive[1] that is integrated in our XP Screens. It was shown to improve crystal quality and resolution by:

- binding to the protein surface and forming tight crystal lattice contacts[3-7]
- acting as linker in various orientations and thereby creating either smaller (PDB: 4OUA) or larger (PDB: 4PHI) protein-protein distances[3,4]
- heterogeneous crystallization of two different protein forms in one single crystal (PDB: 4OUA)[4]
- inducing new crystal forms with access to the active site (PDB: 6ZDK, 6ZDL, 6ZFA)[5]
- covalently binding and structurally adapting to fit into protein molecules (PDB: 4Z12, 4Z13)[2]

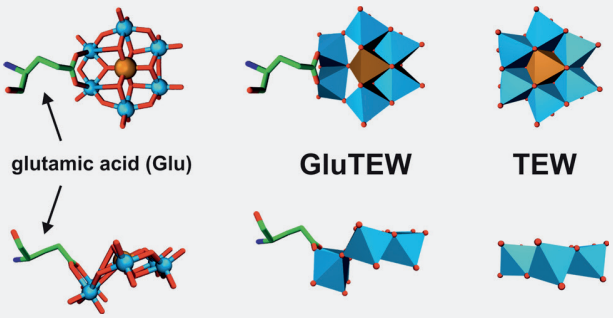

Figure 1: Covalent binding of Tungsten to carboxylic oxygen atoms of glutamic acid (PDB: 4Z12, 4Z13).[2] Figure from [1].

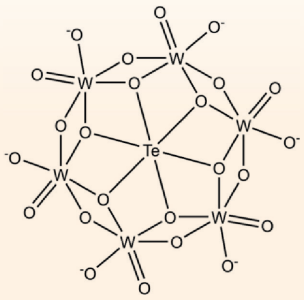

Figure 2: Chemical structure of TEW. Figure from [7].

TEW Properties

- Centrosymmetric, inorganic cluster
- Disk-shaped ion $[TeW_6O_{24}]^{6-}$
- Dimensions: 9 x 9 x 3 Å^3
- MW: 1.615 g/mol (ion)
- Highly soluble in aqueous solutions (100 mM) and stable over a wide pH range
- 6 tungsten atoms provide strong anomalous scattering signal for phasing

References:

[1] Bijelic *et al.* (2017) Ten Good Reasons for the Use of the Tellurium-Centered Anderson-Evans Polyoxotungstate in Protein Crystallography. *Acc. Chem. Res.* **50**:1441.

[2] Molitor *et al.* (2016) *In situ* formation of the first proteinogenically functionalized [TeW6O24O2(Glu)]7- structure reveals unprecedented chemical and geometrical features of the Anderson-type cluster. *Chem. Commun.* **52**:12286.

[3] Bijelic *et al.* (2015) Hen Egg-White Lysozyme Crystallisation: Protein Stacking and Structure Stability Enhanced by a Tellurium(VI)-Centred Polyoxotungstate. *ChemBioChem* **16**:233.

[4] Mauracher *et al.* (2014) Latent and active abPPO4 mushroom tyrosinase cocrystallized with hexatungstotellurate(VI) in a single crystal. *Acta Cryst.* D **70**:2301.

[5] Sobala *et al.* (2020) Structure of human endo-α-1,2-mannosidase (MANEA), an antiviral host-glycosylation target. *PNAS* **117 (47)**:29595.

[6] Ames *et al.* (2020) Identifying a Molecular Mechanism That Imparts Species-Specific Toxicity to YoeB Toxins. *Front. Microbiol.* **11**:959.

[7] Mac Sweeney *et al.* (2018) The crystallization additive hexatungstotellurate promotes the crystallization of the HSP70 nucleotide binding domain into two different crystal forms. *PLOS* one **13 (6)**: e0199639.

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