

Workflow and Tools for Crystallographic Fragment Screening at the Helmholtz-Zentrum Berlin

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Materials

Name	Company	Catalog Number	Comments
1µL pipet	Eppendorf	EP3123000012	
12 channel pipet, 100µL	Eppendorf	EP4861000791	
Blow dryer	TH-Geyer	9.106 788	
Crystal containing crystallization plates			Contains crystals to be soaked
Crystallization incubator			Providing constant temperature for crystallization experiment, at HZB: 20°C
Dual Thickness MicroLoops (LD) of different aperture sizes	MiTeGen	various, e.g. M5-L18SP-75LD	250 loops in the appropriate size needed for the protocol, can be provided by HZB
EasyAccess Frame	HZB		The EasyAccess Frame is a special device for handling multiple crystals, which was developed at the HZB (Barthel et al., 2021).
F2X-Entry Screen plate	HZB		Developed F2X-Entry Screen (Wollenhaupt et al., 2020)
Glas spot plate	VWR	MARI1406506	
Liquid nitrogen			At least a filled up 5 L can
Liquid nitrogen storage can	n.a.	n.a.	
Magentic crystal wand	MiTeGen	M-R-1013198	
Microscopes	Leica	n.a.	
MRC 3-lens 96well low profile crystallization plate	SwissCI	3W96TLP-UVP	For mock-soaked crystals (optional)
Reagent reservoir	Carl Roth	EKT6.1	25 ml volume

Sample tracking template			Provided from HZB, see supplementary information
Scalpel	B. Braun	BA825SU	
Sealing foil for microtiter plates	GreinerBioOne	676070	
Shelved puck shipping canes (for Unipucks)	MiTeGen	M-CP-111-065	2 canes made of aluminum; can be provided by the HZB
Soaking solution			At least 5 ml are needed
Soaking solution including cryo-protectant, 150 μ L			Only needed if soaking solution is not cryo-protectant already
Tissues	Roth (Kimberly Clark Professional)	AA64.1	
Transport dewar (Whartington dry shipper)	MiTeGen	TW-CX100	2 Travel dewars for storage of the 2 unipuck canes, alternatively a storage dewar of type VHC35 or similar could be used.
Unipuck foam dewars with lid	MiTeGen	M-CP-111-022	two foam dewars especially suited for unipuck handling described in the protocol if SPINE pucks are used, different foam dewars might have to be applied.
Unipuck starter set	MiTeGen	M-CP-UPSK001	Can be provided by the HZB
Unipucks	MiTeGen	M-CP-111-021	14 unipucks; can be provided by the HZB