

Materials List for:

Combining Chemical Cross-linking and Mass Spectrometry of Intact Protein Complexes to Study the Architecture of Multi-subunit Protein Assemblies

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Materials

Name	Company	Catalog Number	Comments
Chemicals, Reagents, Consumables			
2-[4-(2-hydroxyethyl)piperazin-1-yl]ethanesulfonic acid (HEPES)	Sigma Aldrich	H4034	buffer
Acetic acid	Sigma Aldrich	695092	pH
Acetonitrile Optima LC/MS	Fisher Chemicals	A955-1	solvent
Amicon Ultra centrifugal devices (different MWCO)	Millipore	i.e. UFC500396	buffer exchange, concentration
Ammonium acetate solution	Sigma Aldrich	A2706	native MS
Ammonium bicarbonate	Sigma Aldrich	9830	in-gel digestion
Ammonium solution	Sigma Aldrich	9859	pH
Bis(Sulfosuccinimidyl)suberate-d0 (BS3-d0)	Thermo Scientific	21590	cross-linker
Bis(Sulfosuccinimidyl)suberate-d4 (BS3-d4)	Thermo Scientific	21595	cross-linker
Caesium iodide	Sigma Aldrich	203033	calibration
Calcium chloride	Sigma Aldrich	C5670	in-gel digestion
Capillaries (1.0 OD × 0.78 ID × 100 L mm)	Harvard Apparatus	30-0038	native MS
Disuccinimidyl suberate (DSS)	Thermo Scientific	21655	cross-linker
DL-Dithiothreitol	Sigma Aldrich	D5545	in-gel digestion
DMSO (dimethyl sulfoxide)	Sigma Aldrich	D8418	solvent
Ethanol	Fisher Chemicals	BP2818	solvent
Formic acid Optima LC/MS	Fisher Chemicals	A117-50	solvent supplement
Instant Blue Coomassie staining solution	expedon	ISB1L	staining solution for gel electrophoresis
Invitrogen NuPAGE 4-12% Bis-Tris gels (1 mm, 10 well)	life technologies	NP0323BOX	gel electrophoresis
Iodoacetamide	Sigma Aldrich	I1149	In-gel digestion
Isopropyl alcohol, HPLC grade	Fisher Chemicals	P750717	solvent
Methanol	Fisher Chemicals	A456-212	solvent
Micro BioSpin 6 columns	BioRad	732-6222	buffer exchange
NuPAGE Antioxidant	invitrogen	NP0005	running buffer, gel electrophoresis
NuPAGE LDS Sample Buffer (4 ×)	invitrogen	NP0007	sample loading buffer (non-reducing) for gel electrophoresis

NuPAGE MES SDS Running buffer	life technologies	NP0001	gel electrophoresis
NuPAGE MOPS SDS Running buffer	life technologies	NP0001	gel electrophoresis
NuPAGE Sample Reducing Agent (10 ×)	invitrogen	NP0004	reducing Agent for gel electrophoresis
PBS - phosphate buffered saline	Sigma Aldrich	P4417	buffer
SeeBlue Plus2 Prestained Standard Protein Marker	invitrogen	LC5925	prestained Protein Marker for gel electrophoresis
Sodium acetate	Sigma Aldrich	S2889	ethanol precipitation
Tris(hydroxymethyl)aminomethane (Tris)	Sigma Aldrich	252859	buffer
Trypsin	Sigma Aldrich	TRYPSEQ-RO (11418475001)	in-gel digestion
Vivaspin centrifugal devices (different MWCO)	Sartorius	i.e. VS0101	buffer exchange, concentration
Water for HPLC	Sigma Aldrich	270733-2.5L-M	solvent
Name	Company	Catalog Number	Comments
Instruments			
Centrifuge Heraeus Fresco 21, bench-top centrifuge	Thermo Scientific	75002425	
Flaming / Brown Micropipette puller Model P-1000	Sutter Instruments	P-1000	
Gelelectrophoresis chamber Xcell SureLock MiniCell	Invitrogen	EI0001	
Gold Coater Quorum Q150R S	Quorum Technologies Ltd.	Q150RS	
Horizontal gel shaker Rotamax 120 T	Heidolph Instruments	544-41200-00	
Q-TOF Ultima mass spectrometer, MS Vision high mass upgrade	Waters (Micromass)	-	
reversed-phase C18 analytical column Acclaim PepMap (C18, 75 mm I.D., 50 cm, 3 mm pore size)	Thermo Scientific	164570	
reversed-phase C18 pre-column (C18, 150 mm I.D., 2 cm, 5 mm pore size)	Thermo Scientific	164213	
scalpel	Fisher Scientific	10463989	
SpeedVac SPD121P vacuum centrifuge	Thermo Scientific	SPD121DP-230	
Thermomixer C	Eppendorf	5382000015	
Tweezers AA	Sigma Aldrich	Z680184-1EA	
Ultrasonic cleaner USC-TH, sonication bath	VWR	142-0084	
UltiMate Dionex 3000 nano-LC system, coupled to Q-Exactive plus hybrid mass spectrometer (nano-ESI source)	Thermo Scientific	0726030+	
Name	Company	Catalog Number	Comments
Software, Software Tools, Database search			
Mascot	www.matrixscience.com		
Massign	http://massign.chem.ox.ac.uk		
MassLynx	Micromass		
MassMatrix	Xu, H. J Proteome Res. 9 (2010)		

MaxQuant	Cox, J. Nat. Biotechn. 26 (2008)		
pLink	Yang, B. Nat Methods 9 (2012)		
pXtract conversion tool	http://pfind.ict.ac.cn/downloads.html		
UniDec	Marty, M.T. Anal. Chem. 87 (2015)		
XCalibur	Thermo Scientific		
XiNET	http://crosslinkviewer.org		
XLinkX	Liu, F. Curr Op Struct Biol 35 (2015)		
xQuest	Rinner, O. Nat Methods 5 (2008)		
Xvis	https://xvis.genzentrum.lmu.de		