

Materials List for

Millisecond Hydrogen/Deuterium-Exchange Mass Spectrometry for the Study of Alpha-Synuclein Structural Dynamics Under Physiological Conditions

Neeleema Seetaloo¹, Jonathan J. Phillips¹

¹Living Systems Institute, Department of Biosciences, University of Exeter

Corresponding Author

Jonathan J. Phillips
jj.phillips@exeter.ac.uk

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Materials

Name	Company	Catalog Number	Comments
1 × 100 mm ACQUITY BEH 1.7 μm C18 column	Waters Corporation	186002346	Analytical column
Acetonitrile HPLC grade>99.9% HiPerSolv	VWR	20060.420	For LC mobile phases
CaCl ₂	Sigma Aldrich	C5670	Salt for HDX buffers
Chronos	Axel Semrau (Purchased from Waters Corporation)	667006090	Scheduling software to enable multiple HDX-MS sample injections automatically. Alternative software is available from other vendors e.g. HDXDirector or LEAP Shell
Deuterium chloride	Goss Scientific (Cambridge Isotope Laboratories)	DLM-2-50	For HDX labelling buffers
Deuterium oxide (99.9% D ₂ O)	Goss Scientific (Cambridge Isotope Laboratories)	DLM-4	Deuterated water
DynamX 3.0	Waters Corporation	176016027	Isotopic assignment and deuterium incorporation calculation
Enzymate BEH Pepsin Column	Waters Corporation	186007233	Pepsin digestion column
Formic Acid, 99.0% LC/MS Grade	Fisher Scientific	10596814	For LC mobile phases
Guanidinium hydrochloride	Sigma Aldrich	RDD001-500G	Chaotrope/Denaturant
HDfleX	University of Exeter	N/A	https://ore.exeter.ac.uk/repository/handle/10871/127982
KCl	Sigma Aldrich	P3911	Salt for HDX buffers
LEAP HDX-2 CTC PAL sampling robot	Waters Corporation	725000637	Autosampler robot
Leucine enkephalin	Waters Corporation	186006013	For mass spectrometry lockspray calibration.
MassLynx	Waters Corporation	667004007	Software controlling inlet methods and mass spectrometer
Maximum recovery vials	Waters Corporation	600000670CV	100 pack including caps - used for quench tray in LEAP HDX-2

MgCl ₂	Sigma Aldrich	M8266	Salt for HDX buffers
Millipore 0.22 µm syringe filters	Millipore	N9CA7069B	Syringe filters
ms2min	Applied Photophysics Ltd	N/A	fast-mix quench-flow millisecond hdx instrument
NaCl	Sigma Aldrich	S9888	Salt for HDX buffers
Peltier temperature controller	LEAP Technologies Inc.	HP115-COOL/D	Peltier controller to set precise temperature of chambers in the LEAP robot.
ProteinLynx Global Server 3.0	Waters Corporation	715001030	Peptide identification software. Alternative software is available from other vendors.
Reagent pot caps	Waters Corporation	186004632	100 pack
Reagent pots for LEAP HDX-2	Waters Corporation	186001420	100 pack excluding caps - used for buffers in LEAP HDX-2
Sodium deuterioxide (99.5% in D ₂ O)	Goss Scientific (Cambridge Isotope Laboratories)	DLM-57	For HDX labelling buffers
Spin filter microcentrifuge tubes (3 kDa MWCO)	Amicon (Merck Sigma Aldrich)	UFC5003	Micro centrifuge tubes to concentrate protein. This facilitates buffer exchange and accurate sample loading for HDX-MS experiments.
Synapt G2-Si mass spectrometer	Waters Corporation	176850035	Mass spectrometer
Total recovery vials	Waters Corporation	600000671CV	100 pack including caps - used for labelling tray in LEAP HDX-2
Tris-HCl	Sigma Aldrich	T3253-250G	Buffer
Trizma base	Sigma Aldrich	T60040-B2005	Buffer
Urea	Sigma Aldrich	U5378-1KG	Chaotrope/Denaturant
VanGuard 2.1 x 5 mm ACQUITY BEH C18 column	Waters Corporation	186004623	Trap desalting column