

Materials List for:

# Synthesis and Structure Determination of $\mu$ -Conotoxin PIIIA Isomers with Different Disulfide Connectivities

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## Materials

Name	Company	Catalog Number	Comments
PS PEG2000 Fmoc Rink-amide Resin	Varian, Inc.	PL3867-3764	AmphiSpheres 40 RAM
Pyr(Boc)	Bachem	A-3850	
Arg(Pbf)	Iris Biotech	FSC1010	
Asn(Trt)	Bachem	B-1785	
Asp(tBu)	Iris Biotech	FSP1020	
Hyp(tBu)	Iris Biotech	FAA1627	
Lys(Boc)	Bachem	B-1080	
Ser(tBu)	Iris Biotech	FSC1190	
Gln(Trt)	Iris Biotech	FSC1043	
Glu(tBu)	Iris Biotech	FSP1045	
Trp(Boc)	Iris Biotech	FSC1225	
Tyr(tBu)	Sigma Aldrich	47623	
Thr(tBu)	Iris Biotech	FSP1210	
His(Trt)	Iris Biotech	FDP1200	
2-(1H-Benzotriazol-1-yl)-1,1,3,3-tetramethyluroniumhexafluorophosphat	Sigma Aldrich	8510060	Flammable
DMF	Fisher Scientific	D119	Flammable, Toxic
DCM	Fisher Scientific	D37	Carcinogenic
Piperidine	Alfa Aesar	A12442	Flammable, Toxic, Corrosive
N-Methyl-Morpholin	Sigma Aldrich	224286	
Cys(Acm)	Iris Biotech	FAA1506	
Cys(Trt)	Bachem	E-2495	
Cys(tBu)	Bachem	B-1220	
trifluoroacetic acid	Sigma Aldrich	74564	Toxic, Corrosive
phenol	Merck	1002060	Toxic
thioanisol	Alfa Aesar	A14846	
ethanedithiol	Fluka Analytical	2390	
diethyl ether	VWR	100,921	Flammable
tert-butanol	Alfa Aesar	L12338	Flammable
acetonitrile	Fisher Scientific	A998	Flammable
water	Fisher Scientific	W5	
isopropanol	VWR	ACRO42383	Flammable
sodium hydroxide	AppliChem	A6579,1000	Corrosive

iodoacetamide	Sigma Aldrich	I6125	
iodine	Sigma Aldrich	I0385	
Hydrochloric acid	Merck	110165	Corrosive
ascorbic acid	Sigma Aldrich	A4403	
diphenylsulfide	Sigma Aldrich	P35405	
anisole	Sigma Aldrich	96109	Flammable
trichloromethylsilane	Sigma Aldrich	M85301	Flammable
sample dilution buffer	Laborservice Onken		
sodium dihydrogen phosphate	Sigma Aldrich	106370	
disodium hydrogen phosphate	Sigma Aldrich	795410	
(2-carboxyethyl)phosphine hydrochloride	Sigma Aldrich	C4706	
citric acid	Sigma Aldrich	251275	
sodium citrate dihydrate	Sigma Aldrich	W302600	
tris-acetate	Carl Roth,	7125	
Ethylenediaminetetraacetic acid	Sigma Aldrich	E26282	
peptide calibration standard II	Bruker Daltonics GmbH	8222570	
Name of Equipment	Company		
solid-phase peptide synthesizer	Intavis Bioanalytical Instruments AG	EPS 221	
lyophilizer	Martin Christ GmbH	Alpha 1-2 Ld <sub>plus</sub>	
semipreparative HPLC	Jasco	system PV-987	
Eurospher 100 C18 column (RP, 5 µm particle size, 100 Å pore size, 250 x 32 mm)	Knauer	25QE181E2J	purification of the linear peptide
Vydac 218TP1022 column (RP C18, 10 µm particle size, 300 Å pore size, 250 x 22 mm)	Hichrom-VWR	HICH218TP1022	purification of the oxidized peptide
analytical HPLC	Shimadzu	system LC-20AD	
Vydac 218TP54 column (C18 RP, 5 µm particle size, 300 Å pore size, 250 x 4.6 mm)	Hichrom-VWR	HICH218TP54	analytical column
ground steel target (MTP 384)	Bruker Daltonics GmbH	NC0910436	MALDI preparation
C18-concentration filter (ZipTip)	Merck KGaA	ZTC18S096	MALDI preparation
MALDI mass spectrometer	Bruker Daltonics GmbH	ultraflex III TOF/TOF	
amino acid analyzer	Eppendorf-Biotronik GmbH	LC 3000 system	
NMR spectrometer Bruker Avance III	Bruker Daltonics GmbH	Bruker Avance III 600 MHz	
computer program for molecular visualising	YASARA Biosciences GmbH	Yasara structures	NMR structure calculation
computer program for MALDI data evaluation	Bruker Daltonics GmbH	flexAnalysis, BioTools	MS/MS fragmentation
analog vortex mixer	VWR	VM 3000	
Microcentrifuge	Eppendorf	5410	
Centrifuge	Hettich	EBA 20	
Rotational vacuum concentrator	Christ	2-18 Cdplus	
Analytical Balance	A&D Instruments	GR-202-EC	