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**Supporting information for article:**

**Overexpression, purification and crystallization of the response regulator NsrR involved in nisin resistance**

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**Protein Analysis  
Molecular Proteomics Laboratory 2014**

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Contact	Sakshi Khosa (AG Schmitt)
Operator	Mareike Brocksieper (mareike.brocksieper@hhu.de)
Sample entry	19.March 2014
Report	16.April 2014
Sample preparation	washing, red./alk. (DTT/ IAA)
Digestion	Trypsin, 37°C, over night
Mass spectrometry	Orbitrap Elite, ESI

**MASCOT-Search**

Database	Swissprot/ extended with the available sequence (below)
Taxonomic	all entries
Enzyme	Trypsin
Missed cleavages	1
Variable modifications	Oxidation (M)
Fixed modifications	Carbamidomethyl (C)
MS tolerance	10 ppm
MS/MS tolerance	0.4 Da

**Sequence:**

NsrR Protein sequence: (Accession no. in the data base: M00016)

MSQEQQKIIYI VEDDMTIVSL LKDHLISASYH VSSVSNFRDV KQEIIIAFPQD LILMDITLPHY  
FNGFYWTAEL RKFLTIPIIF ISSSNDEMDM VMALNMGGDD FISKPFSLAV LDAKLTAILLR  
RSQQFIQQEL TFGGFTLTRE GLLSSQDKEV ILSPTENKIL SILLMHPKQV VSKESSLLEKL  
WENDSFIDQN TLNVNMTRLR KKIVPIGFDY IHTVRCVGYL LQDPNNSSSVD KLAAALEHHH  
HHH

## MS results

### SK1 (OE05640)

MSQEQQK**IYI** VEDDMTIIVSL LKDHLISASYE VSSVSNERDV KQEIIAFQPD LIIMDITLPHY FNGFYWTAEI RKFLLTIPPIF ISSSNDEMMD VMALNMGGDD FISKPPFSLAV LDALKLTAILR RSQQFIQQEL TFGGFTLTRE **GLSSQDKEV** ILSPTENKIL SILLMHPKQV VERESL**IJKL** WENNSFIDQN TLINVNMT**LR** KKEVPIGFDY IHTVRGVGYL LQDPNSSSVD KLAIALEHHHH HHH

Protein	Score	Coverage	#Proteins	# Unique peptides	# Peptides	# PSMs	# AAs	MW [kDa]	Calc. pl
NsrR	26498	49.38 %	1	14	15	2166	243	27.7	6.05

	Identified peptides with high confidence
	Identified peptides with medium confidence
	Identified peptides with low confidence

### Description

Score	Displays the protein score, which is the sum of the scores of the individual peptides.
Coverage	Displays by default the percentage of the protein sequence covered by identified peptides.
# Proteins	Displays the number of identified proteins in the protein group of a master protein.
# Unique Peptides	Displays the number of peptide sequences unique to a protein group.
# Peptides	Displays the number of distinct peptide sequences in the protein group.
# PSMs	Displays the total number of identified peptide sequences (peptide spectrum matches) for the protein, including those redundantly identified.
# AAs	Shows by default the sequence length of the protein.
MW [kDa]	molecular weight
calc. pI	Displays the theoretically calculated isoelectric point, which is the pH at which a particular molecule carries no net electrical charge.