Supplementary Figure 1: MS/MS analysis of isolated *B. fragilis* proteins

Mass spectrometric analyses were performed on an AmaZon ETD ion trap (Bruker Daltoniks, Bremen, Germany) coupled to an Ultimate 3000 UHPLC system (Dionex). The instrument was set up to perform both, CID and ETD fragmentation on the selected precursors. An m/z range from 400-1500 Da was used for data dependant precursor scanning. The three most intense signals in every MS scan were selected for MS/MS experiments, and just signals with a charge state ≥2+ were selected for MS/MS. The data was recorded in the "enhanced resolution mode". Tryptic peptides were separated by reversed phase chromatography (ProteCol™ Capillary Column, SGE, Ringwood, Vic, Australia, 300 µm x 10 mm [precolumn] and 300 µm x 150 mm [analytical column]). The samples were loaded onto the precolumn in 100% solvent A (0.1% Formic acid) and unbound components were eluted by washing the precolumn for 5 min in buffer A. The starting conditions for the analytical column were 2% solvent B (acetonitrile with 0.1% Formic acid). After desalting the sample on the precolumn, a gradient using an increasing solvent B concentration was applied. The gradient conditions were as follows: linear increase of buffer B from 2 to 30% (from 5 min to 61 min), further increase to 60% (61 to 76 min), followed by a steep increase to 90% (76 to 77 min). The column was held at 90% B for 5 min (77 to 82 min) before reequilibrating the analytical column in 2% solvent B. Meanwhile the precolumn was reequilibrated in 100% solvent A before injection of the next sample.

Project Info

Name: David Leitsch **Date:** November 28, 2011

Sample Info & Protocols

Date: August 13, 2013

Name: Bacteroides_II

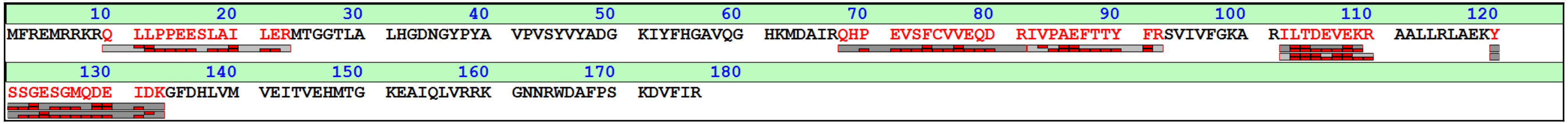
Search Type Combined MS/MS - ProteinExtractor
Search Result Bacteroides_NIM_2013-08-13 15:37:01
Search Location /David Leitsch_Tricho/Bacteroides_II/

Search Type Combined MS/MS - ProteinExtractor
Search Result Amazon Bacteria_NCBI_2013-08-13 13:47:48
Search Location /David Leitsch_Tricho/Bacteroides_II/DL_NimA_RC6_01_560.d/

Protein 1: nimA [Bacteroides vulgatus]

Accession:	gi|435265	**Score:**	461.86
Database:	NCBInr	**MW [kDa]:**	20.20
Seq. Coverage [%]:	35.20 %	**pI:**	7.83
		No. of Peptides:	7

Modification(s): Carbamidomethyl, Oxidation



MFREMRRKRQ LLPPEESLAI LERMTGGTLA LHGDNGYPYA VPVSYVYADG KIYFHGAVQG HKMDAIRQHP EVSFCVVEQD RIVPAEFTTY FRSVIVFGKA RILTDEVEKR AALLRLAEKY
SSGESGMQDE IDKGFDHLVM VEITVEHMTG KEAIQLVRRK GNNRWDAFPS KDVFIR

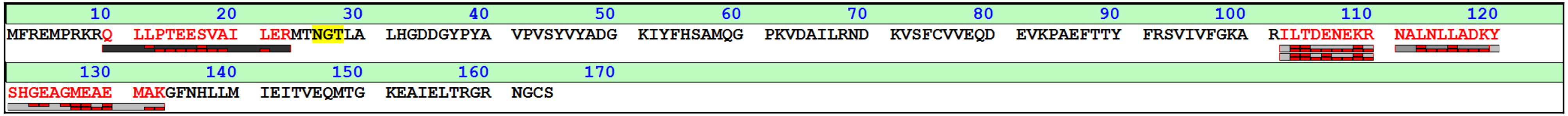
Cmpd.	No. of Cmpds.	m/z meas.	Δ m/z [ppm]	z	Rt [min]	Score	P	Range	Sequence	Modification
250	3	804.4150	-48.22	2	42.9	55.7	0	10-23	R.QLLPPEESLAILER.M	
116	2	865.3480	-62.12	2	31.0	60.0	0	68-81	R.QHPEVSFCVVEQDR.I	Carbamidomethyl: 8
354	4	672.2940	-88.27	2	54.3	62.8	0	82-92	R.IVPAEFTTYFR.S	

Cmpd.	No. of Cmpds.	m/z meas.	Δ m/z [ppm]	z	Rt [min]	Score	P	Range	Sequence	Modification
52	2	473.7070	-108.10	2	24.4	40.5	0	102-109	R.ILTDEVEK.R	
91	4	551.7580	-92.01	2	28.1	77.1	1	102-110	R.ILTDEVEKR.A	
56	1	773.2730	-63.76	2	24.9	50.2	0	120-133	K.YSSGESGMQDEIDK.G	
8	1	781.2970	-29.14	2	19.9	66.3	0	120-133	K.YSSGESGMQDEIDK.G	Oxidation: 8

Search Type Combined MS/MS - ProteinExtractor
Search Result Amazon Bacteria_NCBI_2013-08-13 15:07:52
Search Location /David Leitsch_Tricho/Bacteroides_II/DL_NimD_RC7_01_562.d/

Protein 1: nimD [Bacteroides fragilis]
Accession: gi|440387
Database: NCBInr
Seq. Coverage [%]: 28.00 %
Score: 312.49
MW [kDa]: 18.50
pI: 5.54
No. of Peptides: 5

Modification(s): Oxidation, Deamidated



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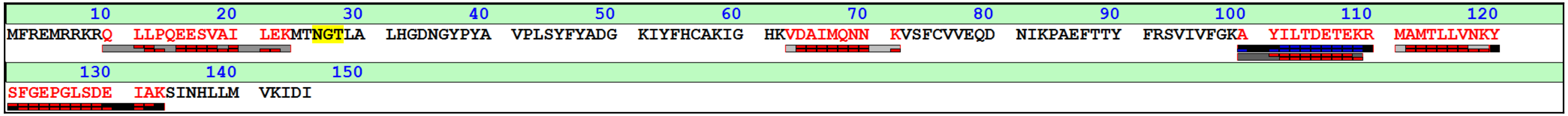
       130        140        150        160        170
SHGEAGMEAE MAKGFNHLLM IEITVEQMTG KEAIELTRGR NGCS
```

Cmpd.	No. of Cmpds.	m/z meas.	Δ m/z [ppm]	z	Rt [min]	Score	P	Range	Sequence	Modification
254	1	799.4130	-38.05	2	39.5	36.6	0	10-23	R.QLLPTEESVAILER.M	
11	1	559.2820	-25.08	2	18.3	68.0	1	102-110	R.ILTDENEKR.N	
16	1	559.7740	-25.07	2	19.0	89.5	1	102-110	R.ILTDENEKR.N	Deamidated: 6
229	10	486.7550	977.53	2	37.3	54.7	0	111-119	R.NALNLLADK.Y	
61	1	504.2060	-17.61	3	22.9	28.8	0	120-133	K.YSHGEAGMEAEMAK.G	

Search Type Combined MS/MS - ProteinExtractor
Search Result Amazon Bacteria_NCBI_2013-08-13 13:05:55
Search Location /David Leitsch_Tricho/Bacteroides_II/NimE2_aus_BA8_01_2798.d/

Protein 1:	NimE nitroimidazole reductase [Bacteroides fragilis]		
Accession:	gi|70559779	**Score:**	397.35
Database:	NCBInr	**MW [kDa]:**	16.60
Seq. Coverage [%]:	39.30 %	**pI:**	8.88
		No. of Peptides:	6
Modification(s):	Oxidation, Deamidated		



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MFREMRRKRQ LLPQEESVAI LEKMTNGTLA LHGDNGYPYA VPLSYFYADG KIYFHCAKIG HKVDAIMQNN KVSFCVVEQD NIKPAEFTTY FRSVIVFGKA YILTDETEKR MAMTLLVNKY
        130        140        150
SFGEPGLSDE IAKSINHLLM VKIDI
```
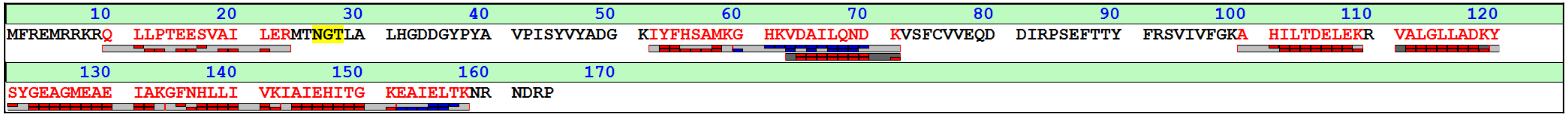

Cmpd.	No. of Cmpds.	m/z meas.	Δ m/z [ppm]	z	Rt [min]	Score	P	Range	Sequence	Modification
125	1	799.0290	104.14	2	39.1	69.1	0	10-23	R.QLLPQEESVAILEK.M	
1	2	525.3440	178.52	2	14.6	57.1	0	63-71	K.VDAIMQNNK.V	Oxidation: 5; Deamidated: 7
61	3	591.8350	62.41	2	26.1	65.3	0	100-109	K.AYILTDETEK.R	
77	7	446.9460	99.56	3	29.0	67.8	1	100-110	K.AYILTDETEKR.M	
48	3	526.8300	99.53	2	23.6	61.3	0	111-119	R.MAMTLLVNK.Y	Oxidation: 1, 3
108	3	756.9460	107.72	2	35.0	76.8	0	120-133	K.YSFGEPGLSDEIAK.S	

Search Type Combined MS/MS - ProteinExtractor
Search Result Amazon Bacteria_NCBI_2013-08-13 13:09:38
Search Location /David Leitsch_Tricho/Bacteroides_II/nimB2_aus_BA3_01_2792.d/

Accumulated Protein Report

Protein 1:	nimB [Bacteroides fragilis]		
Accession:	gi|435261	**Score:**	579.72
Database:	NCBInr	**MW [kDa]:**	18.60
Seq. Coverage [%]:	56.10 %	**pI:**	6.35
		No. of Peptides:	10
Modification(s):	Oxidation		



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MFREMRRKRQ LLPTEESVAI LERMTNGTLA LHGDDGYPYA VPISYVYADG KIYFHSAMKG HKVDAILQND KVSFCVVEQD DIRPSEFTTY FRSVIVFGKA HILTDELEKR VALGLLADKY
SYGEAGMEAE IAKGFNHLLI VKIAIEHITG KEAIELTKNR NDRP
```

Cmpd.	No. of Cmpds.	m/z meas.	Δ m/z [ppm]	z	Rt [min]	Score	P	Range	Sequence	Modification
228	1	799.5420	123.31	2	42.0	28.7	0	10-23	R.QLLPTEESVAILER.M	
89	2	506.8480	194.04	2	24.9	32.4	0	52-59	K.IYFHSAMK.G	Oxidation: 7
142	4	446.6230	102.45	3	31.1	46.0	1	60-71	K.GHKVDAILQNDK.V	
61	3	508.3240	97.26	2	21.6	73.8	0	63-71	K.VDAILQNDK.V	
144	3	584.8810	114.48	2	31.3	64.5	0	100-109	K.AHILTDELEK.R	
174	3	450.3350	118.46	2	34.6	75.8	0	111-119	R.VALGLLADK.Y	
86	3	767.9030	81.87	2	24.5	95.5	0	120-133	K.YSYGEAGMEAEIAK.G	Oxidation: 8
199	5	520.9040	168.58	2	37.2	54.8	0	134-142	K.GFNHLLIVK.I	
120	7	491.3560	134.31	2	28.4	72.5	0	143-151	K.IAIEHITGK.E	
62	2	402.2790	124.07	2	21.8	35.8	0	152-158	K.EAIELTK.N	

Detailed Protein Report

Project Info

Name:	David Leitsch_Tricho	**Date:**	November 28, 2011

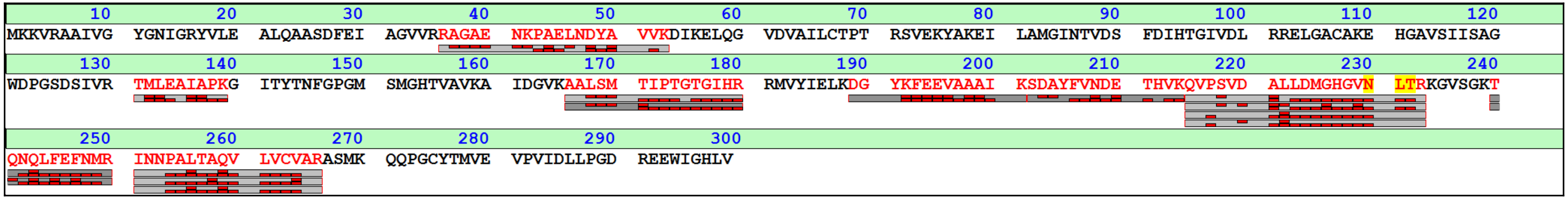
Sample Info & Protocols

		Date:	November 15, 2012
Name:	Bacteroides		

Search Result Info

Search Result	Location	Search Engine	Database	Ident. Compounds
Amazon BFragilis_2012-11-15 18:57:50	/David Leitsch_Tricho/Bacteroides/BF2.mgf	Mascot, 2.3.02	BacteroidesFragilis, uniprotorganismbfragilis.fa	24/290

Protein 1:	Putative oxidoreductase OS=Bacteroides fragilis (strain 638R) GN=BF638R_3505 PE=4 SV=1		
Accession:	E1WVQ6_BACF6	**Score:**	549.06
Database:	BacteroidesFragilis	**MW [kDa]:**	32.30
Seq. Coverage [%]:	63.90 %	**pI:**	6.20
		No. of Peptides:	15
Modification(s):	Carbamidomethyl, Oxidation, Deamidated		



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MKKVRAAIVG YGNIGRYVLE ALQAASDFEI AGVVRRAGAE NKPAELNDYA VVKDIKELQG VDVAILCTPT RSVEKYAKEI LAMGINTVDS FDIHTGIVDL RRELGACAKE HGAVSIISAG
       130        140        150        160        170        180        190        200        210        220        230        240
WDPGSDSIVR TMLEAIAPKG ITYTNFGPGM SMGHTVAVKA IDGVKAALSM TIPTGTGIHR RMVYIELKDG YKFEEVAAAI KSDAYFVNDE THVKQVPSVD ALLDMGHGVN LTRKGVSGKT
       250        260        270        280        290        300
QNQLFEFNMR INNPALTAQV LVCVARASMK QQPGCYTMVE VPVIDLLPGD REEWIGHLV
```

Cmpd.	No. of Cmpds.	m/z meas.	Δ m/z [ppm]	z	Rt [min]	Score	P	Range	Sequence	Modification
50	1	648.9930	-25.33	3	26.2	25.8	1	36-53	R.RAGAENKPAELNDYAVVK.D	

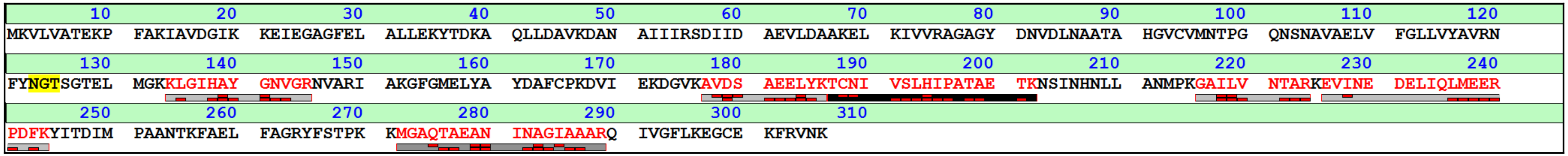
Detailed Protein Report

Cmpd.	No. of Cmpds.	m/z meas.	Δ m/z [ppm]	z	Rt [min]	Score	P	Range	Sequence	Modification
106	3	495.2430	-55.40	2	31.2	44.1	0	131-139	R.TMLEAIAPK.G	Oxidation: 2
124	1	509.2560	-40.63	3	32.9	29.5	0	166-180	K.AALSMTIPTGTGIHR.R	
76	2	514.5670	-80.31	3	28.5	40.3	0	166-180	K.AALSMTIPTGTGIHR.R	Oxidation: 5
146	1	720.8220	-69.50	2	35.2	28.8	1	189-201	K.DGYKFEEVAAAIK.S	
55	1	508.8660	-74.06	3	26.8	25.5	0	202-214	K.SDAYFVNDETHVK.Q	
216	1	1012.0230	491.85	2	42.0	28.9	0	215-233	K.QVPSVDALLDMGHGVNLTR.K	
216	1	1012.0230	5.45	2	42.0	28.9	0	215-233	K.QVPSVDALLDMGHGVNLTR.K	Deamidated: 1
195	2	680.3340	-17.23	3	39.8	63.1	0	215-233	K.QVPSVDALLDMGHGVNLTR.K	Oxidation: 11; Deamidated: 1
195	2	680.3340	465.11	3	39.8	63.6	0	215-233	K.QVPSVDALLDMGHGVNLTR.K	Oxidation: 11
172	1	714.3060	-48.22	2	37.5	22.1	0	240-250	K.TQNQLFEFNMR.I	
130	2	722.2900	-66.31	2	33.7	27.1	0	240-250	K.TQNQLFEFNMR.I	Oxidation: 10
200	1	870.4530	537.64	2	40.2	89.0	0	251-266	R.INNPALTAQVLVCVAR.A	Carbamidomethyl: 13
200	1	870.4530	-27.88	2	40.2	89.0	0	251-266	R.INNPALTAQVLVCVAR.A	Carbamidomethyl: 13; Deamidated: 3
200	1	870.4530	-27.88	2	40.2	89.0	0	251-266	R.INNPALTAQVLVCVAR.A	Carbamidomethyl: 13; Deamidated: 2

Protein 2: Putative D-3-phosphoglycerate dehydrogenase OS=Bacteroides fragilis (strain 638R) GN=serA PE=3 SV=1

Accession:	E1WWI4_BACF6	**Score:**	241.25
Database:	BacteroidesFragilis	**MW [kDa]:**	33.10
Seq. Coverage [%]:	40.20 %	**pI:**	6.17
		No. of Peptides:	6

Modification(s): Carbamidomethyl, Oxidation, Deamidated



```
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MKVLVATEKP FAKIAVDGIK KEIEGAGFEL ALLEKYTDKA QLLDAVKDAN AIIIRSDIID AEVLDAAKEL KIVVRAGAGY DNVDLNAATA HGVCVMNTPG QNSNAVAELV FGLLVYAVRN
       130        140        150        160        170        180        190        200        210        220        230        240
FYNGTSGTEL MGKKLGIHAY GNVGRNVARI AKGFGMELYA YDAFCPKDVI EKDGVKAVDS AEELYKTCNI VSLHIPATAE TKNSINHNLL ANMPKGAILV NTARKEVINE DELIQLMEER
       250        260        270        280        290        300        310
PDFKYITDIM PAANTKFAEL FAGRYFSTPK KMGAQTAEAN INAGIAAARQ IVGFLKEGCE KFRVNK
```
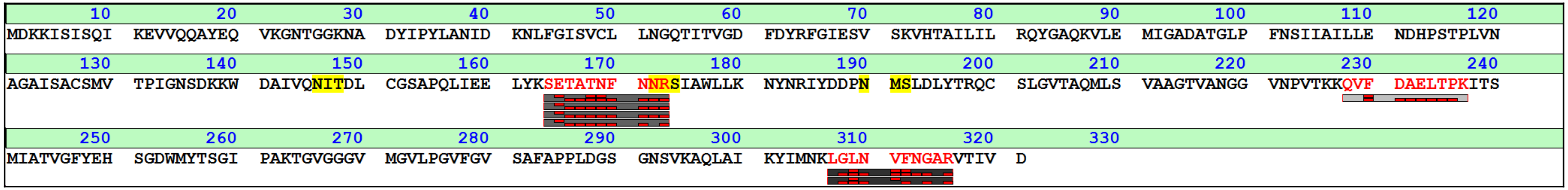

Cmpd.	No. of Cmpds.	m/z meas.	Δ m/z [ppm]	z	Rt [min]	Score	P	Range	Sequence	Modification
30	1	642.8020	-93.65	2	24.6	37.4	1	134-145	K.KLGIHAYGNVGR.N	
53	1	562.7180	-105.08	2	26.5	26.8	0	177-186	K.AVDSAEELYK.T	
127	1	585.6140	-47.30	3	33.3	20.3	0	187-202	K.TCNIVSLHIPATAETK.N	Carbamidomethyl: 2
45	1	457.7430	-68.89	2	25.8	26.5	0	216-224	K.GAILVNTAR.K	
248	1	783.3630	394.12	3	45.1	20.1	0	226-244	K.EVINEDELIQLMEERPDFK.Y	
112	1	865.3940	-48.69	2	31.9	32.1	0	272-289	K.MGAQTAEANINAGIAAAR.Q	

Protein 3: Glutaminase OS=Bacteroides fragilis (strain 638R) GN=glsA PE=3 SV=1

Accession:	E1WKP3_BACF6	**Score:**	173.58
Database:	BacteroidesFragilis	**MW [kDa]:**	34.30
Seq. Coverage [%]:	9.30 %	**pI:**	5.93
		No. of Peptides:	7

Modification(s): Deamidated



```
        10         20         30         40         50         60         70         80         90        100        110        120
MDKKISISQI KEVVQQAYEQ VKGNTGGKNA DYIPYLANID KNLFGISVCL LNGQTITVGD FDYRFGIESV SKVHTAILIL RQYGAQKVLE MIGADATGLP FNSIIAILLE NDHPSTPLVN
       130        140        150        160        170        180        190        200        210        220        230        240
AGAISACSMV TPIGNSDKKW DAIVQNITDL CGSAPQLIEE LYKSETATNF NNRSIAWLLK NYNRIYDDPN MSLDLYTRQC SLGVTAQMLS VAAGTVANGG VNPVTKKQVF DAELTPKITS
       250        260        270        280        290        300        310        320        330
MIATVGFYEH SGDWMYTSGI PAKTGVGGGV MGVLPGVFGV SAFAPPLDGS GNSVKAQLAI KYIMNKLGLN VFNGARVTIV D
```

Cmpd.	No. of Cmpds.	m/z meas.	Δ m/z [ppm]	z	Rt [min]	Score	P	Range	Sequence	Modification
2	1	577.7450	-21.23	2	20.9	23.1	0	164-173	K.SETATNFNNR.S	Deamidated: 6
2	1	577.7450	-21.23	2	20.9	23.4	0	164-173	K.SETATNFNNR.S	Deamidated: 9
2	1	577.7450	-21.23	2	20.9	37.6	0	164-173	K.SETATNFNNR.S	Deamidated: 8
1	1	577.2350	-52.42	2	20.3	51.4	0	164-173	K.SETATNFNNR.S	
108	1	574.2530	-87.62	2	31.5	23.1	0	228-237	K.QVFDAELTPK.I	
161	1	531.2720	-34.91	2	36.3	21.9	0	307-316	K.LGLNVFNGAR.V	Deamidated: 4
161	1	531.2720	-34.91	2	36.3	61.5	0	307-316	K.LGLNVFNGAR.V	Deamidated: 7

Detailed Protein Report

Protein 4: Putative purine nucleoside phosphorylase/uridine phosphorylase family protein OS=Bacteroides fragilis (strain 638R) GN=BF638R_1189 PE=4 SV=1

Accession:	E1WQX2_BACF6	**Score:**	80.95
Database:	BacteroidesFragilis	**MW [kDa]:**	32.30
Seq. Coverage [%]:	7.50 %	**pI:**	5.72
		No. of Peptides:	1

```
        10         20         30         40         50         60         70         80         90        100        110        120
MKKYFPSSEL IINEDGSVFH LHVKPEWLAD KVILVGDPGR VALVASHFEN KECEVESREF KTVTGTYKGK RITVVSTGIG CDNIDIVVNE LDALANIDFQ TREEKEHLRS LELVRIGTCG
       130        140        150        160        170        180        190        200        210        220        230        240
GLQPNTPVGT FVCSEKSIGF DGLLNFYAGR NAVCDLPFER AFLNHMGWSG NMCAPAPYVI DANAELIDRI AQEDMVRGVT IAAGGFFGPQ GRELRVPLAD PKQNDKIEKF EYKGYKITNF
       250        260        270        280        290        300
EMESSALAGL SKLMGHKAMT VCMVIANRLI KEANTGYKNT IDTLIKTVLD RI
```

Cmpd.	No. of Cmpds.	m/z meas.	Δ m/z [ppm]	z	Rt [min]	Score	P	Range	Sequence	Modification
18	1	481.2260	-33.68	2	23.2	61.0	0	190-197	R.IAQEDMVR.G	