



MetaProtServ: Providing a standardized bioinformaticsBiGisolution for metaproteomics data analysis

Fkz 031L0103

Kay Schallert¹, Robert Heyer², Gunter Saake², Dirk Benndorf¹
1 Otto-von-Guericke University Magdeburg, Bioprocess Engineering
2 Otto-von-Guericke University Magdeburg, Chair of Database and Software Engineering

Short description of the project

Targeting cellular functions metaproteomics complements metagenomics and metatranscriptomics as tools widely applied in microbial ecology (e.g. human gut microbiome, biogas plants). Bioinformatics data evaluation in metaproteomics diverges from typical proteomics approaches and faces unique challenges¹. In order to exploit more information from current metaproteome datasets the MetaProteomAnalyzer² (MPA) software was developed. Within MetaProtServ, the GUI based MPA (<u>www.mpa.ovgu.de</u>) [Fig. 1] will be deployed as a powerful web service convincing more scientists from benefits of metaproteomics.

Progress report

We continue to offer the MPA software to the scientific community and constantly grow our user base. Furthermore, we developed the back end for a new fully cloud compliant version of the MPA software³. Currently, the front end for this cloud compliant version is finished. Furthermore, the Prophane software, that offers orthogonal functional and taxonomic annotation, was recently added to the cloud version and is productively deployed on the de.NBI cloud, accessible through www.prophane.de [Fig. 2]. A publication that highlights the combined workflow of MPA and Prophane is currently under review.

					MetaProteomeAnalyzer 2-beta9								E	
Settings Export	Update Help													
Project	🖻 🖻 Proteins (1023)													
	Accession		Description		Taxonomy	SC	MW	pl	PepC	SpC	▼ emPAI	NSAF	w wu	
Input Spectra	🖌 🧔 Q9Y6R7	IgGFc-binding protein	OS=Homo sapiens GN=	FCGBP PE=1 SV=3	Homo sapiens (Species) [9606]	1.67	571.639	5.14	4	7	0.06	0.00011		
	🗸 🎲 Q8EX18	Elongation factor Tu	OS=Mycoplasma penetr	ans (strain HF-2) GN=tuf	. Mycoplasma penetrans HF-2 (Sub	6.85	43.047	6.05	1	7	0.07	0.00153		
	🗸 🏟 A4SCQ7	Elongation factor Tu	OS=Chlorobium phaeovi	brioides (strain DSM 265 .	Chlorobium phaeovibrioides DSM	6.87	42.988	5.19	1	7	0.08	0.00153		
View Results	🔽 🏟 Q6IFZ9	Keratin, type II cytosk	eletal 74 OS=Mus musc	ulus GN=Krt74 PE=3 SV=1	Mus musculus (Species) [10090]	2.42	54.712	5.51	1	6	0.06	0.00104		
	🔽 🍪 P02666	Beta-casein OS=Bos	taurus GN=CSN2 PE=1	SV=2	Bos taurus (Species) [9913]	8.48	25.091	5.26	1	6	0.23	0.00230		
	🔽 🎲 P33048	Beta-casein OS=Capr	ra hircus GN=CSN2 PE=:	2 SV=1	Capra hircus (Species) [9925]	8.56	24.849	5.26	1	6	0.21	0.00233		
	🔽 🎲 Q4FZU2	Keratin, type II cytosk	eletal 6A OS=Rattus no	rvegicus GN=Krt6a PE=1 .	. Rattus norvegicus (Species) [101	1.81	59.213	8.06	1	6	0.05	0.00094		
Logging	🔽 🍪 P11839		aries GN=CSN2 PE=1 S		Ovis aries (Species) [9940]	8.56	24.859	5.26	1	6	0.21	0.00233		
	🔽 🏟 Q9TSI0	Beta-casein OS=Buba	alus bubalis GN=CSN2 P	E=2 SV=1	Bubalus bubalis (Species) [89462]	8.48	25.090	5.26	1	6	0.21	0.00230		
	✓ Sp P51589	Cytochrome P450 2/2	OS=Homo sapiens GN=	-CYP2I2 PE=1 SV=2	Homo sapiens (Species) [9606]	1.99	57.574	8.76	1	6	0.06	0.00103		
	Q4FPN5				Candidatus Pelagibacter ubique	3.57	38.804	9.28	1	6	0.07	0.00154		
	✓ Sp P06872		anis lupus familiaris PE=	-	Canis lupus familiaris (Subspecies	44.13	26.406	4.67	4	6	1.31	0.00209		
	A6KXA0	21			. Bacteroides vulgatus ATCC 8482 (58.107	5.12	3	6	0.16	0.00095		
	P02662		Bos taurus GN=CSN1S1		Bos taurus (Species) [9913]	21.50	24.513	4.98	3	5	0.54	0.00201		
	A5WGK9				. Psychrobacter sp. PRwf-1 (Specie	3.79	43.182	5.02	1	5	0.08	0.00109		
	🖌 🤹 Q9C4Z1	v	· · · · ·		. Methanosarcina thermophila (Sp	12.13	47.154	4.65	2	5	0.19	0.00098		
	018740				. Canis lupus familiaris (Subspecies		76.308	5.65	1	5	0.04	0.00055		
	P07963				Methanococcus vannielii (Species	3.85	29.763	5.68	1	5	0.10	0.00165		
			y							-				
	Q Peptides (1)				Detail Charts								ă.	
	✓ Sequence		ProtC	SpC 🔻 🖽	Biological Process Ontology									
	C A DMPIQAFLLYQEPVLGPVR 4			Methanogenesis										
			Transcription 34 (2,89%)											
			Ion transport 35 (2,98%)											
	Spectrum Matches (6)				Transcription regulation									
	🔍 Spectrum Matches (43 (3.66%)								

MPA-Cloud Prophane						
Job Submission Job Control	About					
1 Input	Input		expert			
	Job label	Yet another Prophane job				
2 Sample Groups	Source	MetaProteomeAnalyzer (MPA)	\$			
3 Quantification	Report file	Metaprotein_FASP_Metagenom.csv	Browse			
4 Taxonomy	FASTA file	Physarum_Transcriptome_Final.fasta	Browse			
	Exclude	accessions starting with				
5 Function						

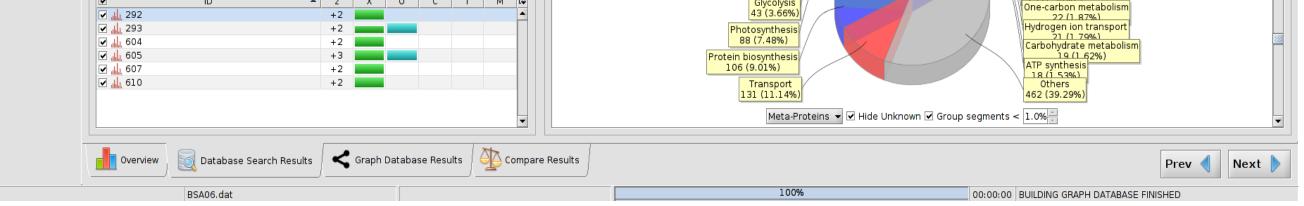


Figure 1: The MPA software provides an intuitive graphical user interface, which enables researchers without a background in bioinformatics to run the data analysis easily.

de.NBI services

The MetaProteomeAnalyzer (MPA) is provided to the research community as a centralized remote server solution and as a download for local installation. Users can access the server and its resources by creating an account. Currently 60 (previous period: 30) individual users are registered, of which at least twenty continuously use the software for their ongoing projects. With respect of the small size of the metaproteomics community this constitutes a major increase in the user numbers. The acquired data volume exceeds 12 TB (previous period: 5).

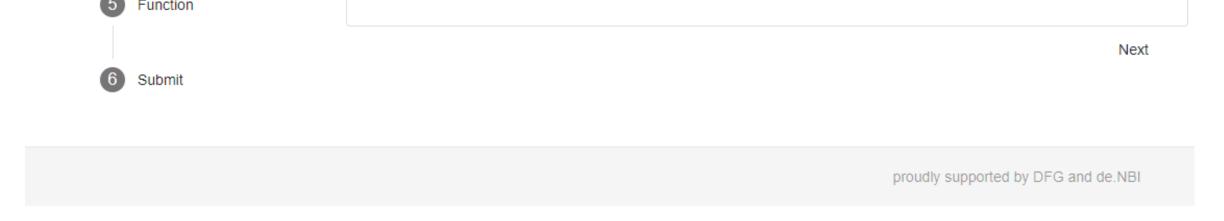


Figure 2: The new MPA-Cloud-Website currently hosted on the de.NBI cloud. The picture shows part of the finished Prophane section of the page, allowing users to submit analysis jobs.

de.NBI Training and education

We gave two official de.NBI courses. The first course was conducted in June over a week, and included a two day laboratory preparation of the participants samples for the following three day MPA software training course. The second course was conducted in September, as part of the GCB2019 conference. It focused on talks on the theoretical background of metaproteomics. Furthermore, users are continuously supported. In addition, the activities of de.NBI will be presented at the 4th International Metaproteome Symposium which is co-organized by Dirk Benndorf as a member if the scientific comittee.

The MetaprotServ partner project currently employs two staff members paid from de.NBI (Kay Schallert and Robert Heyer). Two staff members are project leaders (Dirk Benndorf and Gunter Saake). Furthermore, several staff are involved in consulting (David Broneske, Sebastian Püttker). We also established a industry partnership with Bruker Daltonik GmbH (Heiko Neuweger, Sven Bremer).

Publications

[1] "Challenges and perspectives of metaproteomic data analysis"; R. Heyer & K. Schallert et al. (2017)
Journal of Biotechnology; 261, 24-36, 2017, https://doi.org/10.1016/j.jbiotec.2017.06.1201
[2] "A robust and universal Metaproteomics Workflow for Research Studies and Routine Diagnostics
Within
24 h Using Phenol Extraction EASP Digest and the MetaProteomeAnalyzer": R. Heyer & K. Schallert et al.

24 h Using Phenol Extraction, FASP Digest, and the MetaProteomeAnalyzer"; R. Heyer & K. Schallert et al. (2019)

[3] "MSDataStream - Connecting a Bruker Mass Spectrometer to the Internet "; R. Zoun et al. (2019)Datenbanksysteme f
ür Business, Technologie und Web

