METABOLATOR: Establishing a Citable Web Application for Automated Metabolic Load Analysis

David Pape¹, Mani Lokamani¹, Ayush Seal², Oliver Knodel¹, Jeffrey Kelling³, Karim Fahmy², Guido Juckeland¹

¹ Department of Information Services and Computing | ² Institute of Resource Ecology | ³ Institute of Radiation Physics

1. Introduction and Background



- Biophysics Department at Institute of Resource Ecology studies growth-metabolism relations in microorganisms
- Chemical turnover in metabolizing cells exhibits conserved heat flow patterns in the enthalpy (heat) domain
- Analysis of microcalorimetry data, extraction of characterizing values through curve fitting ("metabolic load" model 10.3390/microorganisms10071397)



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https://metabolator.hzdr.de

	А	В	С	D	E	F	G	AZ
1	February 20, 2024 16:01:04	Room Temperature	Temperature [Temperature]	Heat flow [Signal, Ch 2:1]	Heat [Signal, Ch 2:1]	Normalized heat flow	Normalized heat	Time markers
2	S	°C	°C	W	J	W/g	J/g	
3								
4								
5	-3833.3680832386		30.000000905361					
6	-3832.50313210487		30.000000901552					
7	-3831.6078388691	21.2101373653797	30.000000897609					
8	-3830.45527887344	21.207983173176	30.000000892534	-8.76193629316989E-08				
84	-37.4299716949463	21.5434546836034	29.999998584617	-9.94816032455709E-05				
85	0	21.5695550986244	29.9999990515765	-0.0001438360354897				Reaction start
86	49.2972500324249	21.4899591238178	30.000007203706	-0.000168405843564774				
87	110.464402675629	21.3374438589115	30.0000032055929	-0.000180927515815041				
106	1047.12396192551	21.0382266881895	29.9999995275162	-1.76754310217565E-05				
107	1096.42121195793	21.2533339454881	29.9999990377513	-4.71609660284222E-05				Measuring position
108	1145.71846175194	21.3259258640943	30.000004134717	-6.61930059628266E-05				
159	3659.91364002228	21.1972189536172	29.9999997230875	-1.61447544397168E-06				
160	3709.2108900547	21.2020462203285	29.9999997523174	-1.61864906740777E-06				
161	3758.50814008713	21.2062506623082	29.9999997815472	-1.62455243492872E-06				Signal correct
162	3807.80539011955	21.2119752171251	29.9999998324154	-1.62228284211317E-06	-8.54017243751092E-05			
163	3857.10526418686	21.2177530675649	29.9999998832868	-1.61950411717652E-06	-0.000165372032063302			
164	3906.40251421928	21.2335681463865	29.999999387631	-1.62345480590909E-06	-0.000245411917485014			



Thermal metabolic power **P(H)** of microbiological culture with characterizing parameters H_0 , H_f , r_0 .

$$P(H) = r_0 \cdot H \cdot \frac{H_0 - H}{H_0 - H + H_f}$$

- Request to Computational Science department:
- -Automation of the analysis to streamline local experimental process
- -Offer analysis as a web service to the microcalorimetry community worldwide

An example dataset as it is currently used. Many rows and columns are hidden to aid visualization. Proprietary file formats (e.g. Excel XLS) are often used; data layout varies between datasets.



2. Concept and Design of the METABOLATOR Tool

- Fixed set of features and inputs and outputs
- Users can analyze own datasets \rightarrow common data exchange format required
- User interface based on initial Jupyter Notebook created by student assistant
- Execution and presentation of the notebook as a website using Voilà
- Implementation using typical Python data science libraries and frameworks





NETAE nalysis of M you use META	BOLATOR licrocalorimetric Metabolic Dat BOLATOR for your data analysis, pl	ta Using Monod's Equation	DOI 10.3390/microorganisms10071397 DOI 10.14278/rodare.3050 DOI 10.14278/1e4y-rc46	
. Dataset sele	ction		2. Select Ranges	3. Plot and Analyze
Srowse freeded the	Heat flow [Signal, Ch 2:1], W Heat flow [Signal, Ch 2:2], W Heat flow [Signal, Ch 2:2], W Heat flow [Signal, Ch 2:3], W Heat flow [Signal, Ch 2:4], W Heat flow [Signal, Ch 2:5], W		Time Offset 15000 Power Offs 0 Heat Rang 0.05 – 0 Estimate Heat Range Check Offsetting	Enthalpy Plot Time Plot 14 Analyze Data / Fit Download: Test_NCTC_Gluc_Lac_20022024_clean_analysis.xlsx Test_NCTC_Gluc_Lac_20022024_clean Heat flow [Signal, Ch 2:1], W Heat range selection: [0.05, 0.1399999999999999999] Fitted interval: [0.05070389, 0.13604858]
50	0.2 0.4 0.6	0.8 1 1.2	1.4 1.6	r_sq: 0.99941865 rz: 364.48082605 +/- 3.92754065 delta: 0.03304251 +/- 0.00096425 hz: 0.17458772 +/- 0.00072150 hf: 0.00260573 +/- 0.00016845 Pmax: 50.18009116 Hmax: 0.12183149

An initial draft of the tool and its features sketched on a whiteboard.



plotly 🦳 Jupyter

Software DOI 10.14278/rodare.3049

3. Implementation

Implementation follows FAIR Principles for Research Software (FAIR4RS):

- Published on Rodare, harvested by B2FIND (F, A)
- Understandable, well-structured code (R)
- High code quality through automated tests and static code analysis in CI (R)
- Installable Python library (R)
- Permissive, open source license; explicitly stated (R)
- Data exchange format for interoperability?



A variety of tools and services was used to ensure FAIRness according to the FAIR4RS principles.

4. Service Provision





An overview of the METABOLATOR publications and their relations to each other (using the DataCite 4.4 vocabulary). To avoid visual clutter, the "supplement" relations are only shown in one direction. The inverse relations (e.g. "METABOLATOR Software is supplemented by METABOLATOR Service") exist as well.

- Hosted at HZDR, available worldwide
- Service citable via DOI registered with DataCite and interlinked with other publications
- Academic credit for providers of software and service



The module structure of the METABOLATOR application. Python modules are blue, the Jupyter Notebook is gray. The three modules on top provide building blocks used by the app module which implements the GUI. The GUI is instantiated in the Jupyter Notebook run with Voilà.



Establishing a data exchange format in the community allows for metadata to be considered as well.

DataCite Fabrica	About Support			
10.14278/1e4y-rc4	16			
	URL	XXIIJSBU		
	https://metabolator.hzdr.de/	INTERNATIONAL SOCIETY FOR		
Metadata Export DataCite XML	Metadata			
DataCite JSON Schema.org JSON-LD	METABOLATOR Web Application Service	UUNFEKENUE I		
BibTeX	David Pape, Lokamani, Ayush Seal, Oliver Knodel, Jeffrey Kelling, Karim Fahmy, Guido Juckeland, Service published 2024 via Helmholtz-Zentrum Dresden-Rossendorf	MEXICO CITY		
DOI registered March 27, 2024 at 13:05:26	L https://doi.org/10.14278/1e4y-rc46	28-31 OCTOBER 2024		
UTC	Citation			
July 29, 2024 at 06:53:11 UTC	Pape, David, Lokamani, Ayush Seal, Oliver Knodel, Jeffrey Kelling, Karim Fahmy, and Guido Juckeland. "METABOLATOR Web Application." Helmholtz-Zentrum Dresden-Rossendorf, 2024. https://doi.org/10.14278/1E4Y-RC46.	The service will be presented to the international micro-		
		calorimetry community in October.		



Department of Information Services and Computing · Computational Science Department

David Pape · d.pape@hzdr.de · https://www.hzdr.de/fwcc-d



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