

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

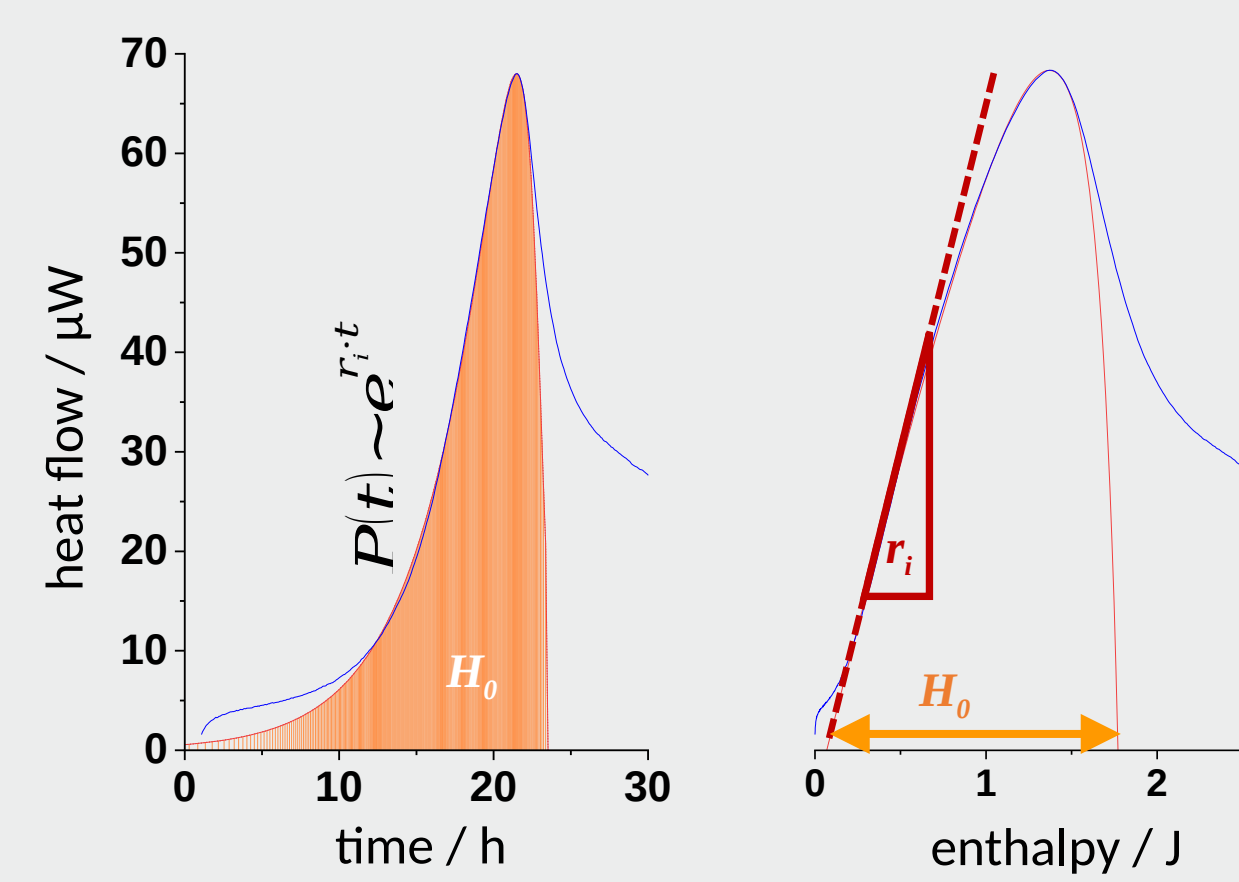
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<https://metabolator.hzdr.de>

1. Introduction and Background



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

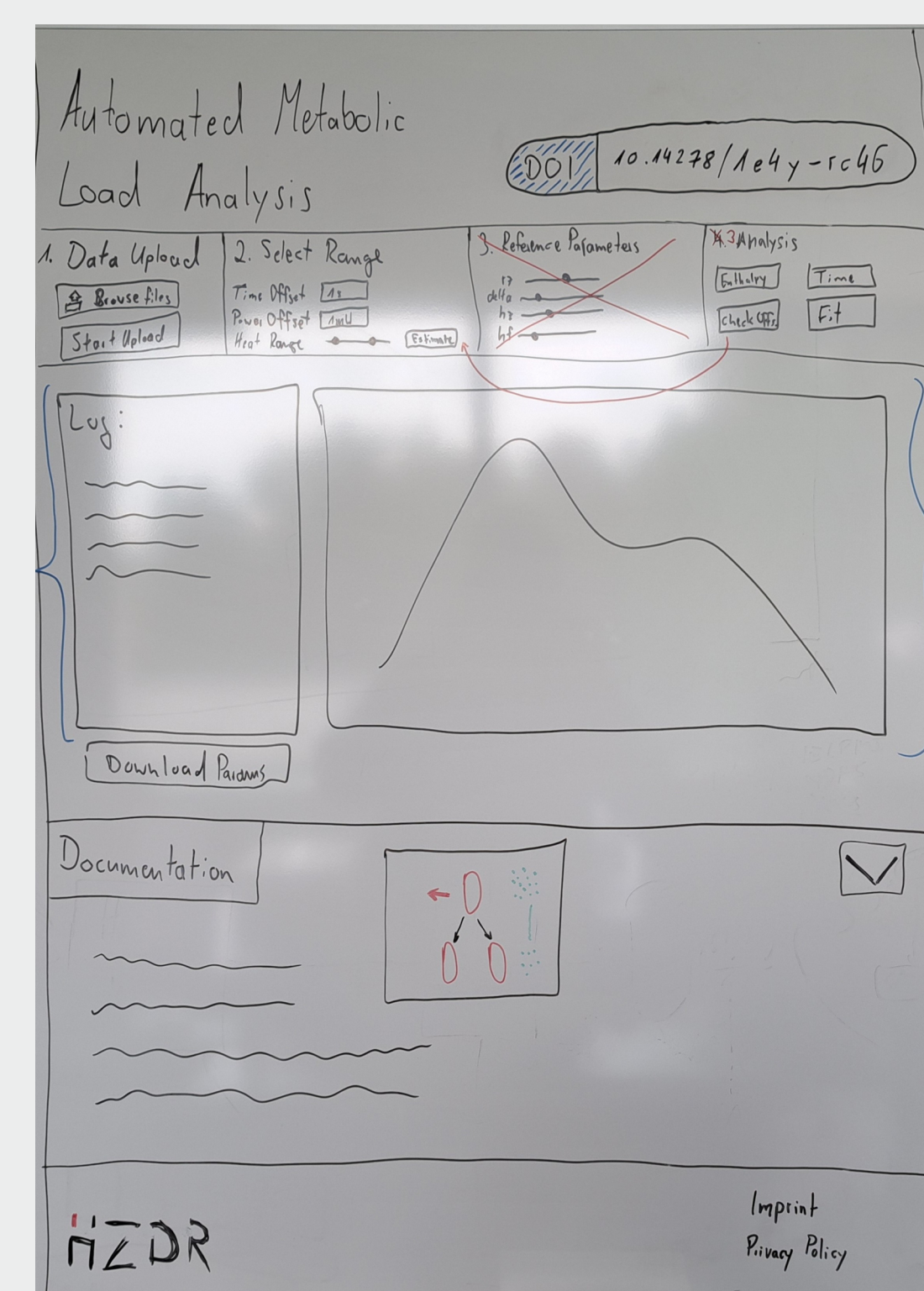
$$P(H) = r_0 \cdot H \cdot \frac{H_0 - H}{H_0 - H + H_f}$$

- 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](https://doi.org/10.3390/microorganisms10071397))
- 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

	A	B	C	D	E	F	G	AZ
1	February 20, 2024 16:01:04	Room Temperature	Temperature	Heat flow	Heat	Normalized	Normalized	
2		°C	[Temperature]	[Signal, Ch 2:1]	[Signal, Ch 2:1]	heat flow	heat	Time markers
3			°C	W	J	W/g	J/g	
4								
5								
6	-3833.3680832386		30.0000000905361					
7	-3832.50313210487		30.0000000901552					
8	-3831.6078388691	21.2101373653797	30.0000000897609					
9	-3830.45527987344	21.207983173176	30.0000000892534	-8.76193629316989E-08				
10	-37.4299716949463	21.5434546836034	29.999999584617	-9.94018023455709E-05				
11		0	21.569550986244	29.999999515765	-0.0001438360354897			Reaction start
12	49.2972500324249	21.4899591238178	30.0000007203706	-0.000188405843564774				
13	110.464462078629	21.3374438589115	30.0000002055929	-0.000189297151815041				
14	1047.12396192551	21.038226881895	29.9999995275162	-1.7675410217565E-05				Measuring position
15	1098.421121195793	21.2533339454881	29.9999990377513	-4.71609660284222E-05				
16	1145.71846175134	21.3259259640943	30.0000004134717	-6.8193059628266E-05				
17	3659.91364022238	21.1972189536172	29.9999997230675	-1.6144754397168E-06				
18	3709.210900547	21.2020462203285	29.9999997523174	-1.61864906740777E-06				
19	3768.50814008713	21.2062506623082	29.9999997815472	-1.62455243482972E-06				Signal correct
20	3807.80539011995	21.2119752112551	29.9999998341554	-1.62228284211317E-06				
21	3857.10526418686	21.2177530675649	29.9999998832868	-1.61950411717652E-06	-8.54017243751092E-05			
22	3906.40251421928	21.2335681463865	29.9999999387631	-1.62345480909090E-06	-0.000245411917485014			

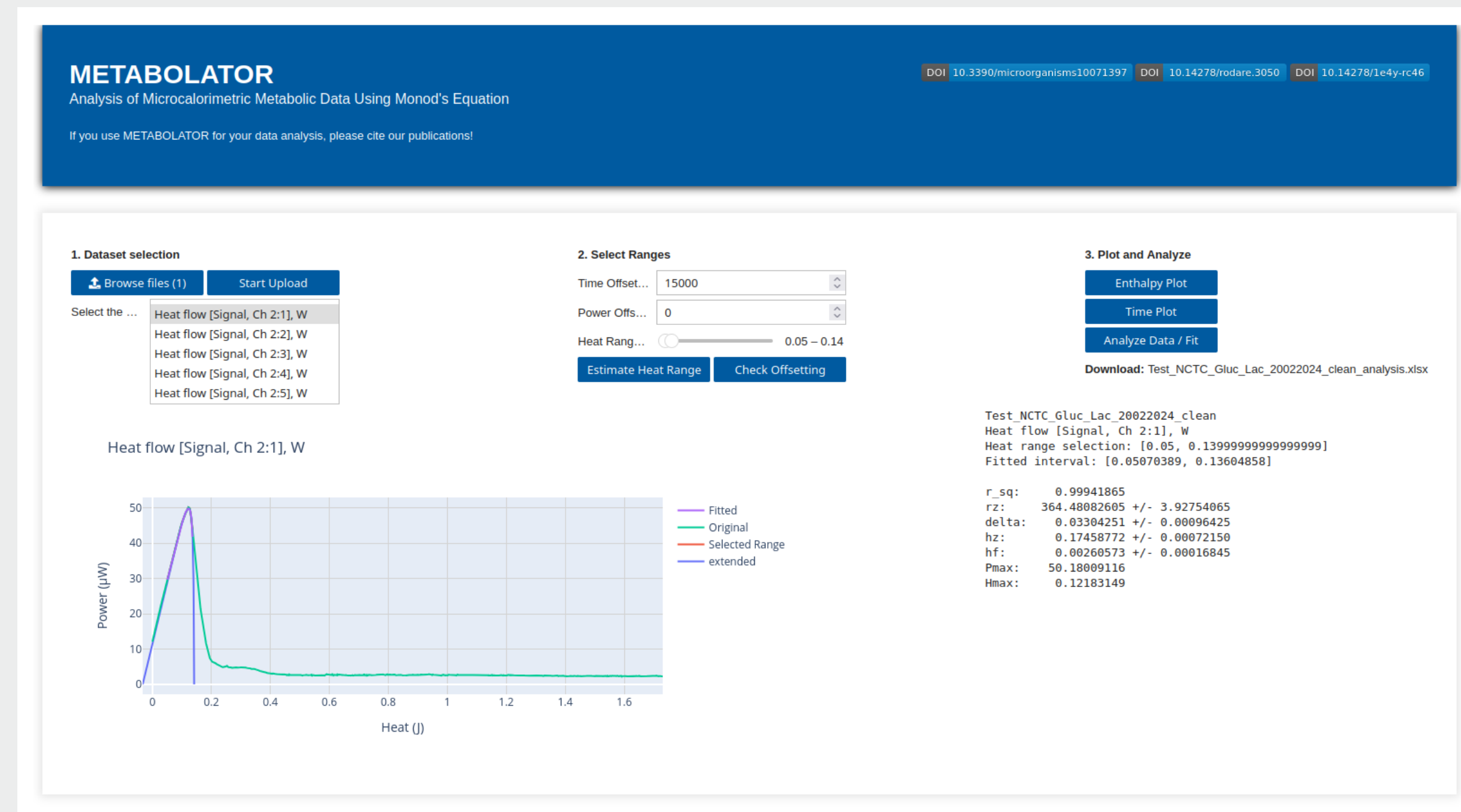
An example dataset as it is currently used. Many rows and columns are hidden to aid visualization. Proprietary file formats (e.g. Excel XLS) are often used; data layout varies between datasets.

2. Concept and Design of the METABOLATOR Tool



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

- Fixed set of features and inputs and outputs
- Users can analyze own datasets → **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



A screenshot of the current implementation.

3. Implementation

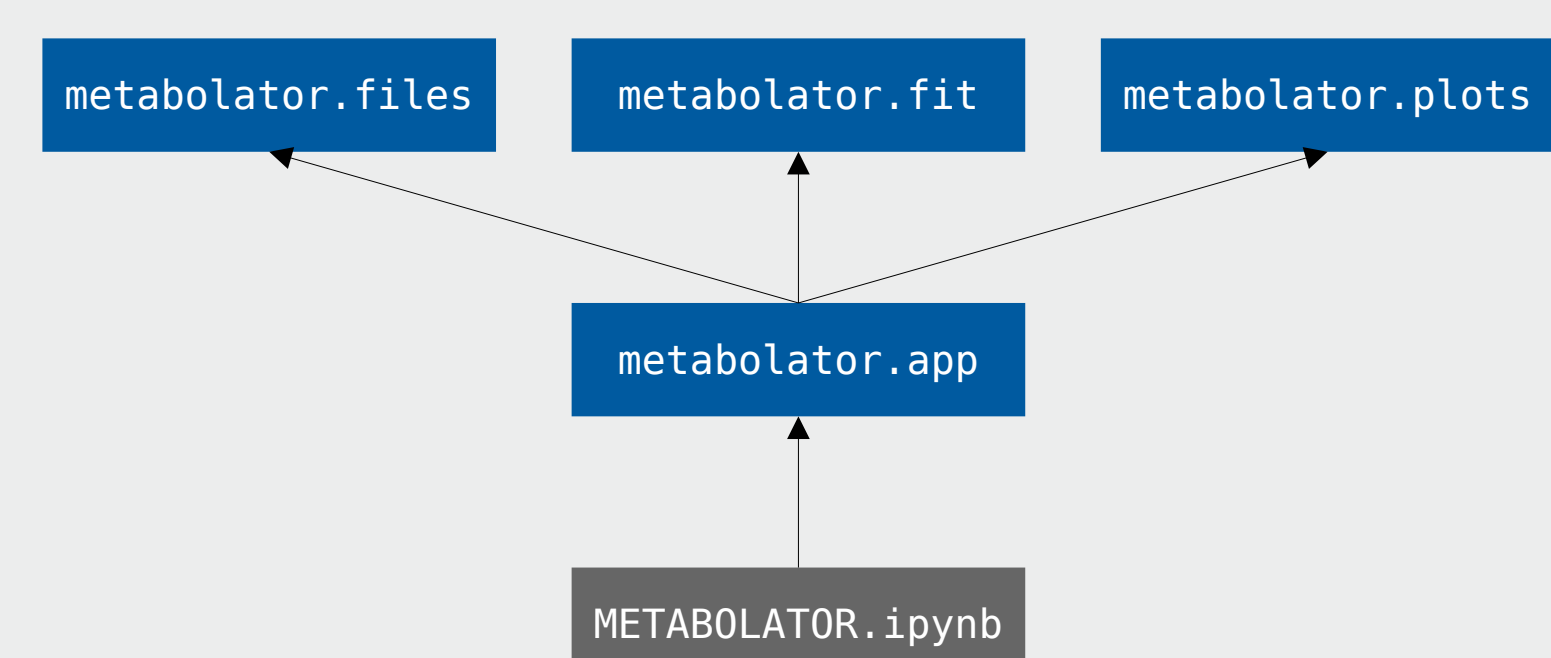
Implementation follows **FAIR Principles for Research Software (FAIR4RS)**:

- 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?**

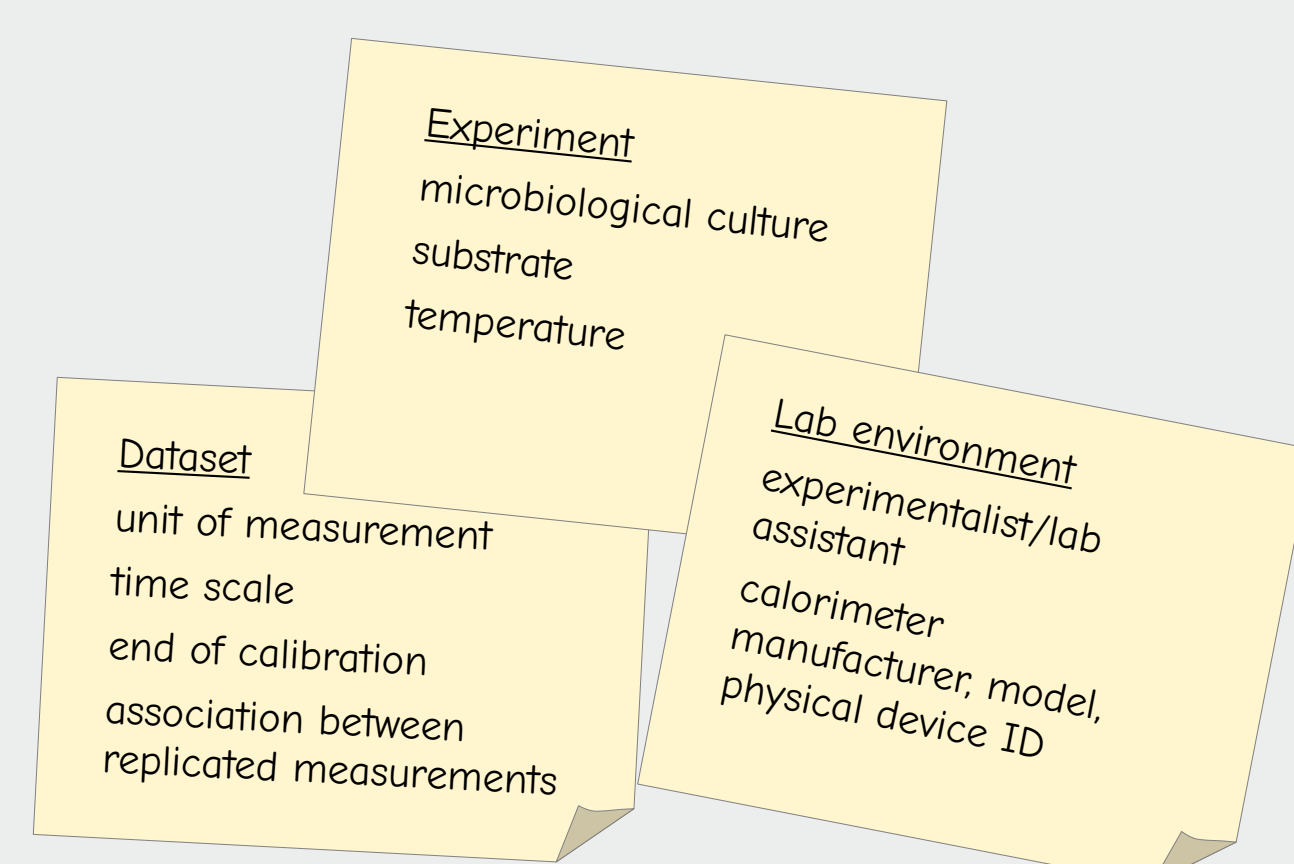
Software DOI [10.14278/rodare.3049](https://doi.org/10.14278/rodare.3049)



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



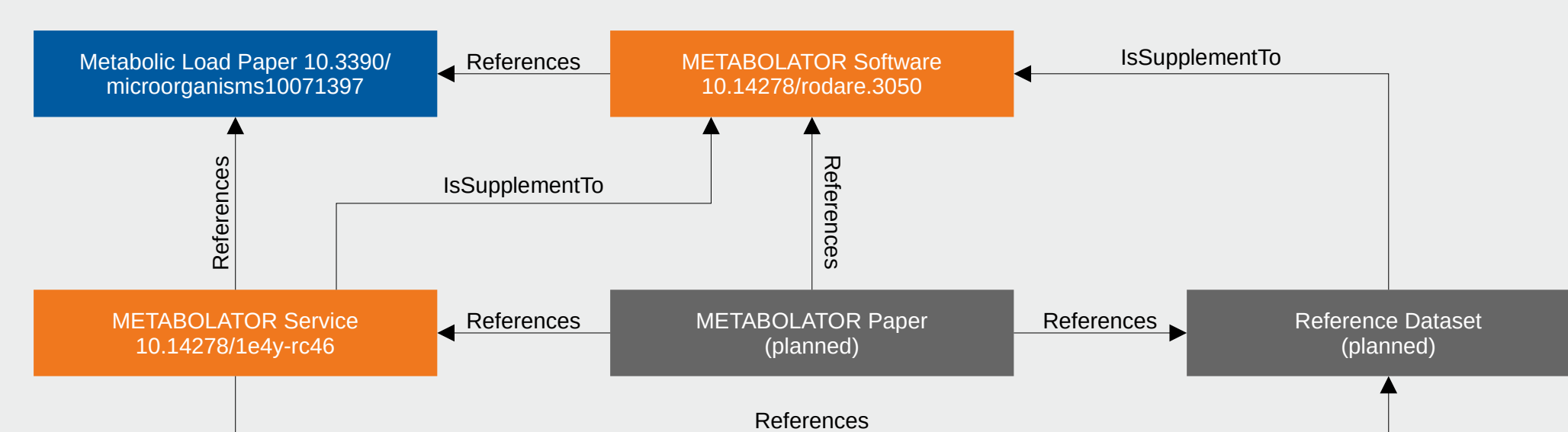
The module structure of the METABOLATOR application. Python modules are blue, the Jupyter Notebook is gray. The three modules on top provide building blocks used by the app module which implements the GUI. The GUI is instantiated in the Jupyter Notebook run with Voilà.



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

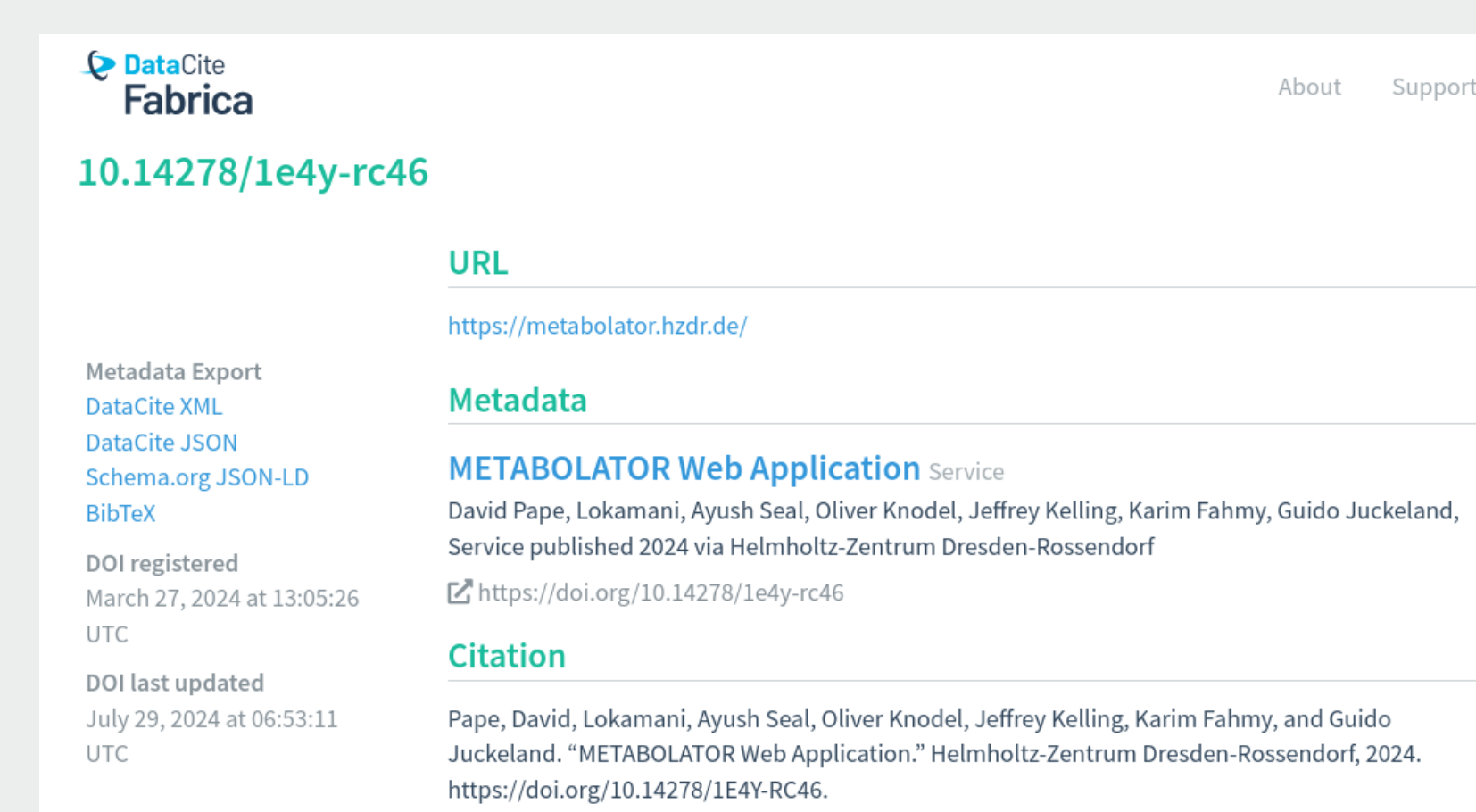
4. Service Provision

Service DOI [10.14278/1e4y-rc46](https://doi.org/10.14278/1e4y-rc46)



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 service will be presented to the international microcalorimetry community in October.