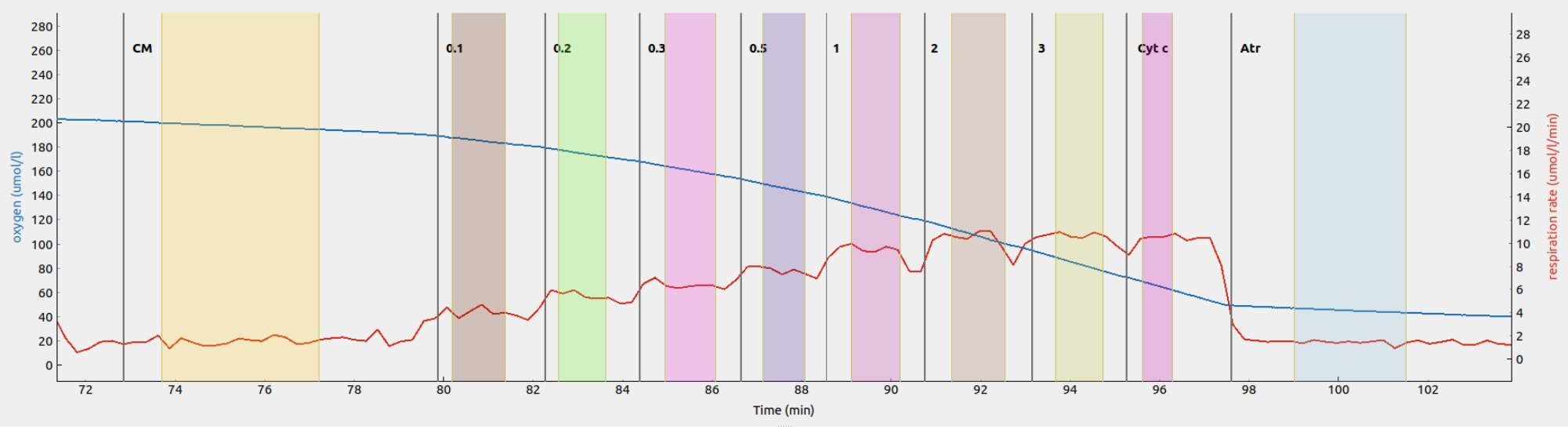
Platform for Primary Kinetics Data Analysis

Martin Laasmaa

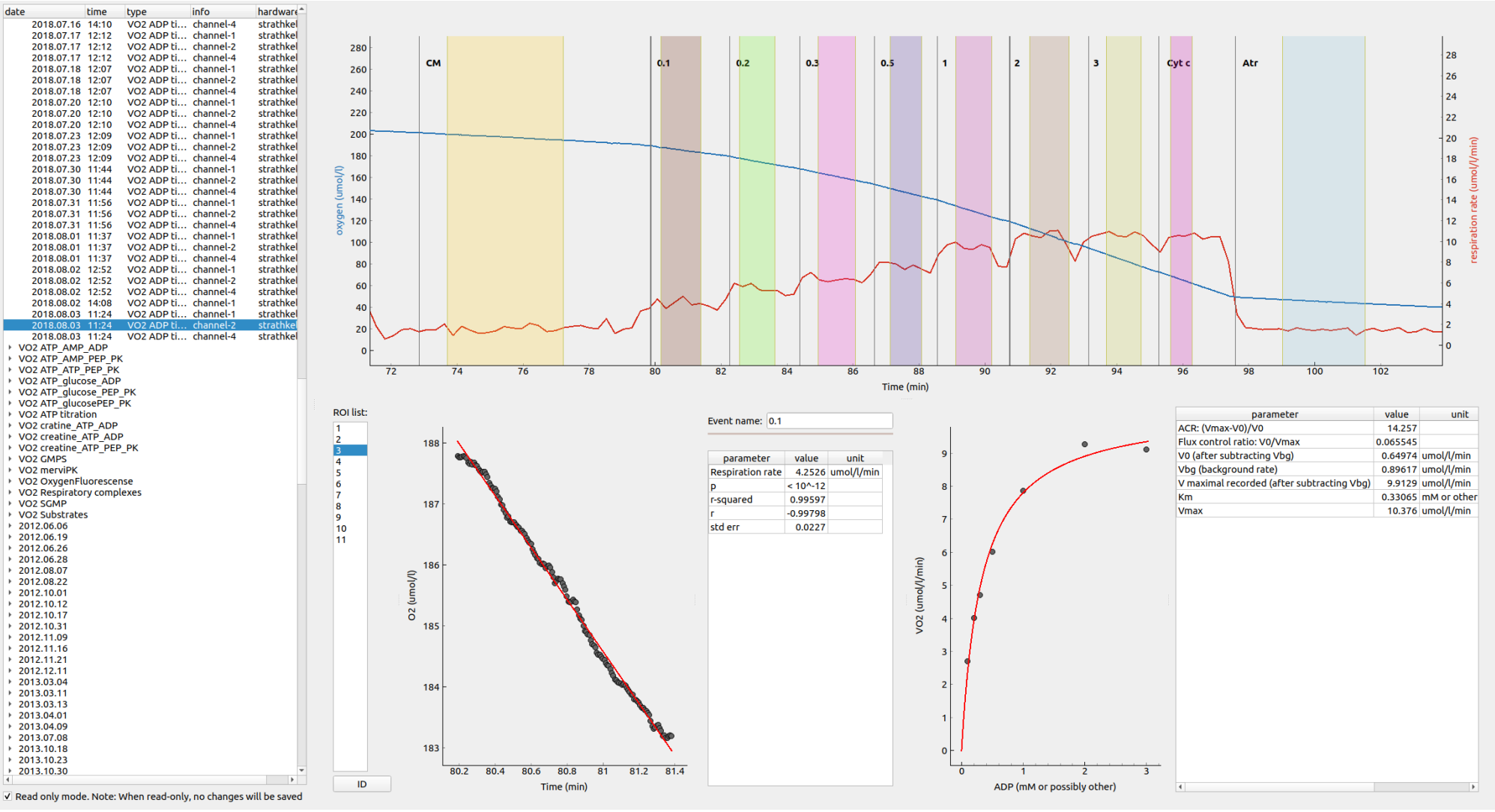
Laboratory of Systems Biology
Department of Cybernetics
School of Science
Tallinn University of Technology



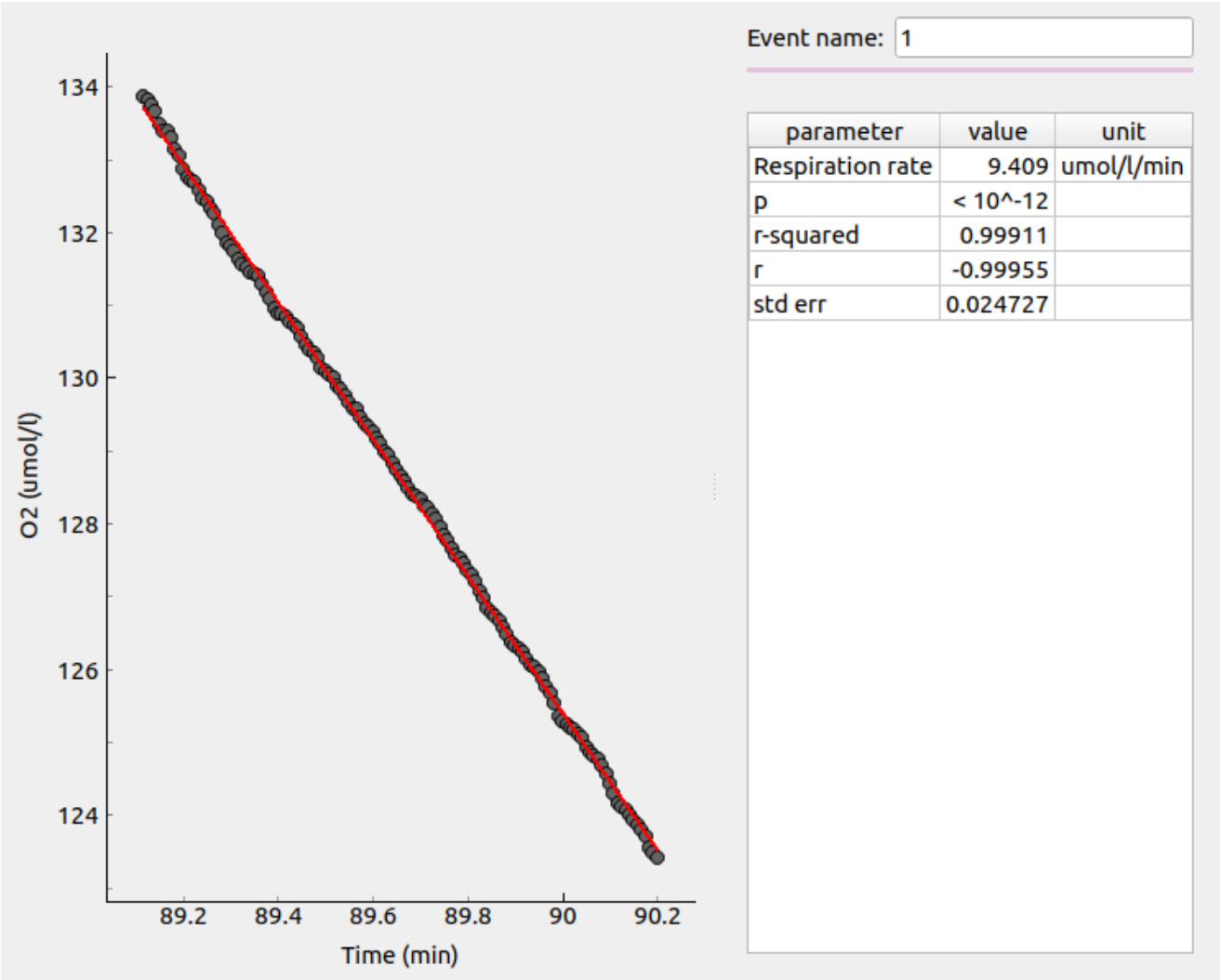
Motivation

- Consistency
  - multiple researchers
  - students
- Simplicity
  - data review
  - data normalization
  - data processing
- Viability
  - publishing
  - collaboration

An example of respiration kinetics experiment

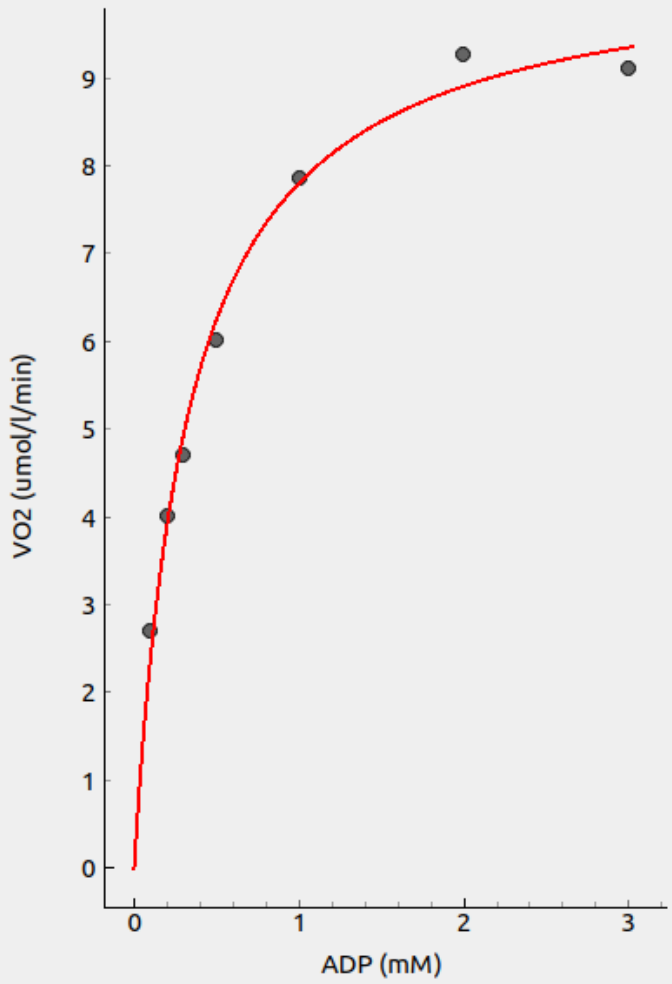


An example of respiration kinetics experiment (2)



parameter	value	unit
Respiration rate	9.409	umol/l/min
p	< 10^-12	
r-squared	0.99911	
r	-0.99955	
std err	0.024727	

An example of respiration kinetics experiment (3)



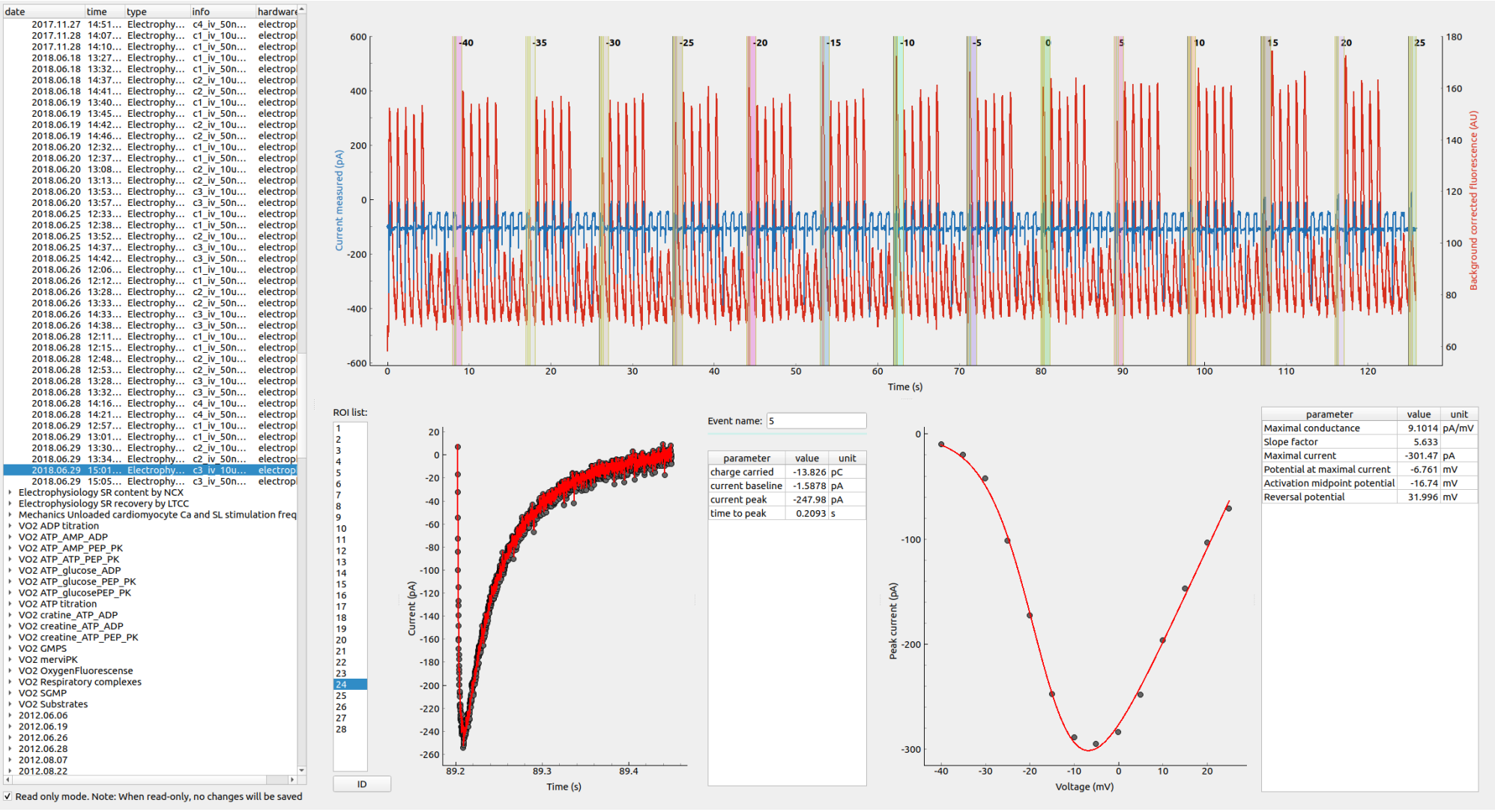
parameter	value	unit
ACR: (Vmax-V0)/V0	14.257	
Flux control ratio: V0/Vmax	0.065545	
V0 (after subtracting Vbg)	0.64974	umol/l/min
Vbg (background rate)	0.89617	umol/l/min
V maximal recorded (after subtracting Vbg)	9.9129	umol/l/min
Km	0.33065	mM
Vmax	10.376	umol/l/min

An example of respiration kinetics experiment (4)

date	time	type	info	hardware
2018.08.03	11:24	VO2 ADP ti…	channel-1	strathkelvin
2018.08.03	11:24	VO2 ADP ti…	channel-2	strathkelvin
2018.08.03	11:24	VO2 ADP ti…	channel-4	strathkelvin

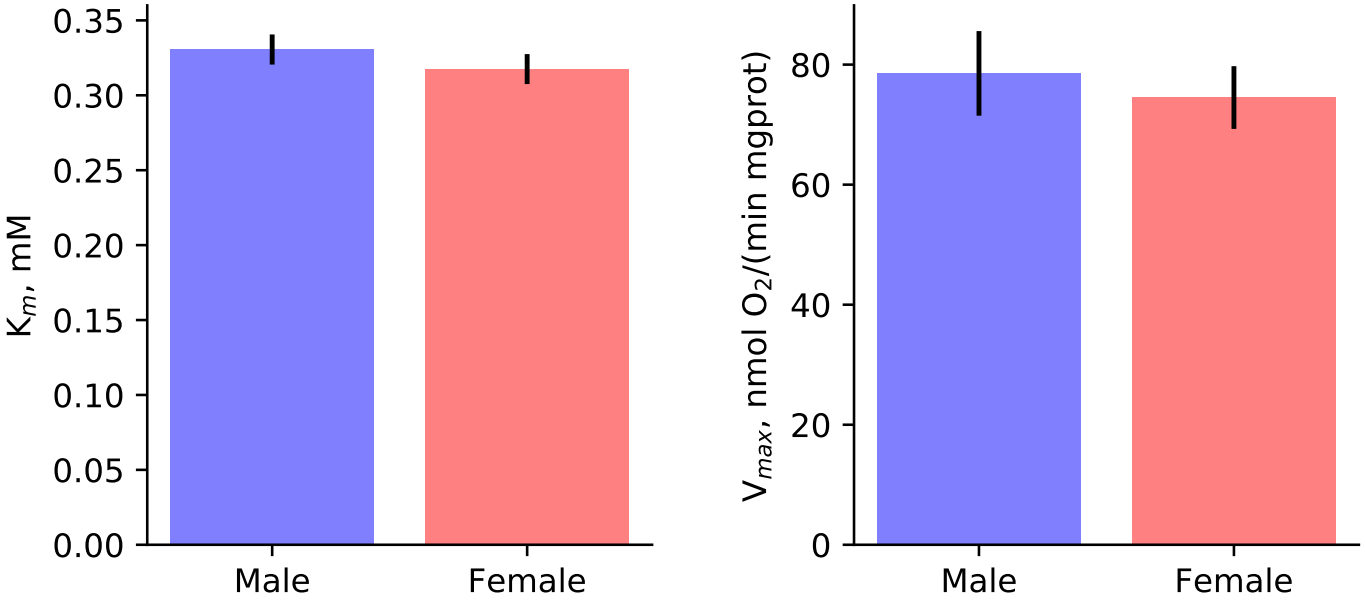
- VO2 ATP_AMP_ADP
- VO2 ATP_AMP_PEP_PK
- VO2 ATP_ATP_PEP_PK
- VO2 ATP_glucose_ADP
- VO2 ATP_glucose_PEP_PK
- VO2 ATP_glucosePEP_PK
- VO2 ATP titration
- VO2 creatine_ATP_ADP
- VO2 creatine_ATP_PEP_PK
- VO2 GMPS
- VO2 merviPK
- VO2 OxygenFluorescense
- VO2 Respiratory complexes
- VO2 SGMP
- VO2 Substrates
- 2012.06.06
- 2012.06.19
- 2012.06.26
- 2012.06.28
- 2012.08.07
- 2012.08.22
- 2012.10.01
- 2012.10.12

An example of patch clamp experiment



Getting data

```
SELECT km, vmax, sex
FROM kinetics_vo2_adp_titration_mm_normalized
WHERE spid = 'mouse C57BL6 generic'
```



Kinetics software schema

Software is designed in modular fashion

- **IO:**
  - Raw data readers: Strathkelvin, spectrometer, electrophysiology, ...
  - Database backend: SQL
- **Analyzers:**
  - library: linear regression, Michaelis–Menten kinetics, spline fitting, integration
  - primary: VO_2, electrical current properties / charge
  - secondary: VO_2 Michaelis–Menten, IV-curve fitting
- **Protocols:** ADP/ATP titration, L-type calcium current, ...

Software stack

Our platform has following components:

- kinetics software
- database with our schema and frontend. Supporting:
  - PostgreSQL for institutional use (server)
  - SQLite for personal use (PC)
- SQL tools for getting data for:
  - visualization
  - statistical analysis
  - mathematical modeling

Database schema

Database consists of different tables:

- animals
- chemicals
- solutions
- preparation
- experiments
- studies
- ...

Linking animal's history from its genetic heritage with experimental results

Database frontend

Preparation: Preparation Animal mouse

Preparations: mice>Edit 1574 / 2018-03-22 09:44:10

BACK VIEW Muscles CM isolations

Id	332
Animal	1574 / mouse C57BL6 generic
Preparation prepared	2018-03-22 09:44:10 Time at which preparation was ready
Weight	22.00 Weight of animal [g]
Appearance	Healthy Appearance of an animal
Tibial Length	2.16 Tibial length [cm]
Comments	Isolation - Martin & Marko

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Database frontend (2)

Isolations: Mouse cardiomyocytes

CM isolations>Edit 273 / 2018-03-22 09:45:01

BACK | VIEW | Pump | Pressure | Solutions | Cardiomyocytes

Id	273
Isolation started	2018-03-22 09:45:01 Time at which you started isolation
Preparation Animal	1574 / 2018-03-22 09:44:10 Animal used as a source for isolation
Thermostat Temperature	38.50 Thermostat temperature during isolation [C]
Initial Pressure	14.20 Initial pressure [mmHg]
Initial Flow	2.20 Initial flow [ml/min]
Post Incubation Time	45.00 Time in post-incubation [min]
Post Incubation Temperature	38.50 Temperature during post-incubation [C]
Comments	All went well. Heart was nicely digested when taken off.

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Future

We planning to:

- prepare kinetics software for open source release:
  - testing
  - supporting different operating systems
- package server components:
  - self hosting
  - cloud service
  - integration to existing infrastructure

Summary

We developed a platform for primary kinetics data analysis that:

- would be easy to use,
- keeps consistency in the data processing and storing,
- enables quick and easy access to the data by all team members.

We expect that using such approach improve quality of research.

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Contact:

Marko Vendelin:	`markov@sysbio.ioc.ee`
Martin Laasmaa:	`martin@sysbio.ioc.ee`
web:	`sysbio.ioc.ee`