The Netherlands' arm of ISBE-Light
Infrastructure for Systems Biology Europe
ISBE.NL

Make Me My Model For You

Emergence of innovative systems biology: Infrastructure Systems Biology Europe (ISBE)

Dr. Alexey Kolodkin

Infrastructure for Systems Biology Europe (the Netherlands node)

CORBEL

Brussels,
June 20, 2017

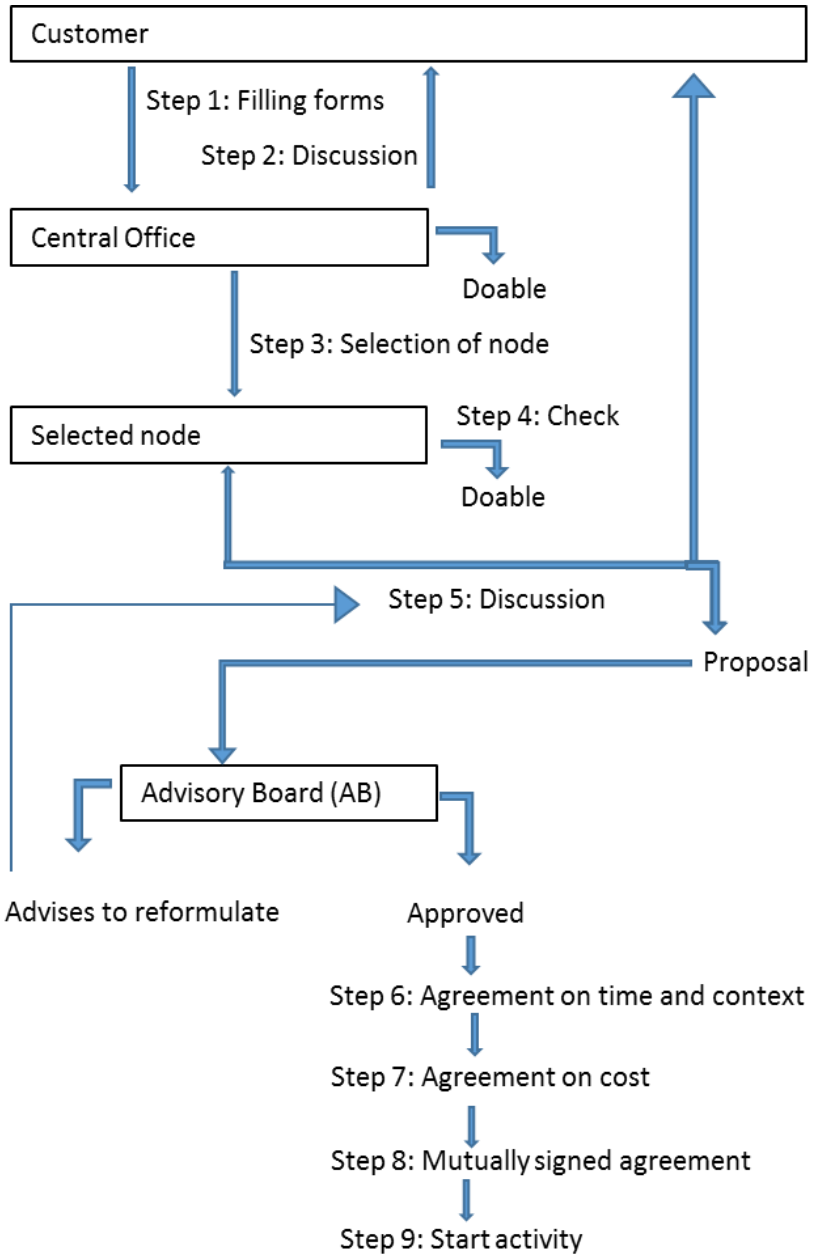
Infrastructure Systems Biology Europe (ISBE) services:

- Make-Me-My-Model (M4)
- Make-Me-My-Experiment
- Teaching (Online computer tutorials)
- Data stewardship (with FAIRDOM)

Make
Me
My
Model
For You

M4 mission:

to service the Life Sciences community by facilitating the implementation of systems biology



Proposed ISBE M4 access management

Check our websites!

http://project.isbe.eu/

services/

Scopus - Document s | Reviewer recognition | MICINN - Sede Electr | CVN | JCR - Journal Citation | MICINN - Sede Electr

ISBELight

About ISBE | Modelling Services | Data Management | Training Services | Events & News

services offered by ISBE

Training Services

Education and training in systems biology is key to ensuring the effective adoption of systems biology approaches to tackle today's academic, societal and industrial challenges. ISBE's ambition is to train a new generation of systems biologists equipped with the cross-disciplinary skills that wi
systems biology- but that also have applications in many areas of academia, gover
consultancy and non-governmental organisations.

The Education and Training module gives researchers access to educational materi
biology and makes them aware of courses, workshops and conferences.

If you would like to add your material to this platform, please email it to m.kalinows

Educational material on Systems Biology

The Systems Biology Educational Portal was developed by ERASysAPP, the ERA-Net for A
aim of the portal is to improve knowledge exchange between Systems Biology researchers
to share their expertise. Furthermore, the intention is for the platform to become a central
material on Systems Biology, for students and lecturers alike. The possibility for users to ev
platform is a great step in this direction.

We would like to invite Systems Biology students, lecturers and researchers to contribute t
platform by posting articles, presentations and lectures relevant to Systems Biology. Users
feedback on the published content, as the evaluation of the posts is an important key succ
Biology Educational Portal.

Graduate study programs

ERASysAPP and ISBE have jointly developed a catalogue of 'Graduate Study Programs'. T
Master's and PhD programmes. The catalogue has filter options to simplify the search for
of the featured programmes focus exclusively on systems biology; whereas, others feature
specialism within an interdisciplinary curriculum. Organisers of relevant study programmes
this overview by submitting programmes which have not yet been listed.

Events & News

Open Call For Ritrain Staff Exchanges

www.isbe.nl

ISBE@NL

Research Infrastructure Systems Biology Europe, NL branch

Welcome to ISBE.NL

The Netherlands' arm of ISBE-Light (the Infrastructure for Systems Biology Europe),

ISBE@NL, has started its operation 1 September 2016, with its first activity: Make Me My Model 4M 4U:

Non modellers can request (assistance with) the making of a computational model of their biological system

ISBE-light and ISBE@NL have a booth/exhibition at the ICSB2016 in Barcelona, where Dr Alexey Kolodkin will be eager to address your questions and to establish ideas about models to be made.

A future activity will be 'Do Me An Experiment' with possibilities to have enzyme kinetics and epigenetics experiments done quantitatively.

If interested, please e-mail:

Alexey Kolodkin (a.n.kolodkin@vu.nl) or Hans V. Westerhoff (H.V.Westerhoff@uva.nl)

The Netherlands arm of the Infrastructure Systems Biology Europe (ISBE):

The Netherlands' arm of ISBE-Light Infrastructure for Systems Biology Europe

ISBE.NL

Alexey Kolodkin, Matteo Barberis, Ablikim Abdukerim, Zahid Hassan, Thierry Mondeel, Samrina Rehman and Hans V. Westerhoff

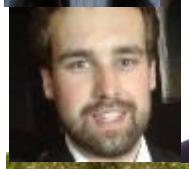
executive director

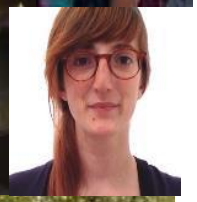
founding director

Stefania Astrologo, Ewelina Weglarz-Tomczak , YanFei Zhang, Jacky Snoep

- Executive director Dr Alexey Kolodkin (UvA, VU, LCSB, Corbel)
- Postdoctoral fellow Dr Ewelina Weglarz-Tomczak (UvA)
- Part-time help from Westerhoff group members (VUA, UvA, UoM)
- Pending integration with Wageningen (Vitor Martins dos Santos et al)

ISBE.NL expertise





Prof Hans Westerhoff (UvA, VUA, UoM): **dynamic modelling, MCA, non-equilibrium thermodynamics**

Dr Samrina Rehman (UoManchester): **Data analysis for metabolomics and transcriptomics**

Ms Yanfei Zhang (UvA): **Extremophile energetics**

Ms Stefania Astrologo (UvA): **Stochastic modelling mRNA and epigenetics**

Mr Thierry Mondeel (UvA): **Mathematics; cell cycle model, FBA, Microbial energetics**

Dr Zahid Hassan (VUA): **Systems microbiology and bioremediation**

Dr Ablikim Abdukerim (VUA): **Immunology modelling**

Dr Matteo Barberis (UvA): **Cell cycle Modelling**

Prof. Jacky Snoep: data stewardship, modelling, malaria, HIV

Dr. Ewelina Weglarz-Tomczak (UvA): **Modelling for ISBE.NL and personalized medicine, enzyme design**

Dr Alexey Kolodkin (Executive Director of ISBE.NL): **Dynamic modelling of signalling and Parkinson's disease**

ISBE.NL services

The services provided at present

ISBE.NL M4 services (currently running and planned to be completed within the next 12 months and in negotiation phase):

Completed services

1. University of Duisburg-Essen, Germany: Cool design of hot metabolism: GAPN
2. Sanquin, Amsterdam: Modelling of acute and chronic inflammation

Active services

3. LCSB, Luxembourg: ROS management in Parkinson's disease and cancer
4. Milano-Bicocca, Italy: Modelling ROS management and mitochondrial dysfunction
5. Sheffield, UK: Mitochondrial perfect adaptation
6. Lisbon, Portugal: CFTR maturation
7. URV Tarragona, Spain: Safety assessment of endocrine disrupting chemicals
8. Institute of Experimental and Clinical Medicine, Novosibirsk, Russia: Modulation of ROS management by TC13 for Parkinson's disease therapy
9. Universidade Católica Portugues, Portugal: Molecular Insight into Autism Spectrum Disorder (ASD)
10. Jožef Stefan Institute, Slovenia: Protease signaling network in neurodegeneration

Prospective services

11. Munich, Germany: Charged peptide to charged membrane binding model
12. Helmholtz Center Munich, Germany: Modelling substrate diffusion and metabolism in biofilms
13. Institute of Cytology and Genetics of RAS, Novosibirsk Russia: Merged ODE and agent-based model for multilevel integration of signalling pathways
14. Manchester, UK: Modelling fibromatosis (Dupuytren's disease), Chronic Myeloid Leukaemia (CML), and urothelial cancer
15. University of Duisburg- Essen, Germany: The Yin-Yang of Metabolism; Endometatoxicity (YYME)

Current status of ISBE.NL M4 services

		WP 1 setting model idea	WP 2 building network	deliverab Diagram in SBGN	WP3 building mathematical model	milestone first simulations	deliverable working toy model COPASI	WP4 model fitting & improvin	mileston working final model	deliverable model presented to customer	WP5 model analysis	milestone model predictions	deliverable report for customers
Completed services													
1	Essen-GAPN											paper is in press	
2	Sanquin-Inflammation									molel has been presented to customer			
Active													
3	LCSB-ROS												
4	Milan-ATP												
5	Sheffield-Perf Adapt												
6	Lisbon -CFTR												
7	Tarragona Endocrine												
8	Novosib-TC13-NRrf2												
9	Portugal-Autism												
10	Slovenia-Neurodegen												
Prospective													
11	Munich-membrane												
12	Helmholtz-Biofilms												
13	Novosib-signalling												
14	Manchester-Leukaemia												
15	Essen-Endotoxicity												

The FAIRDOMHub Login | The FAIRDOMHub Progr

Secure | https://fairdomhub.org/programmes/27#projects

11 projects (services)

Search here... | Search | + | Alexey Kolodkin

Home / Programmes Index / Model repository for M4 (Make Me My Model) clients of ISBE

Model repository for M4 (Make Me My Model) clients of ISBE

Administration

ISBE-Light provides M4 service (Make Me My Mode) where non modelers can request (assistance with) the making of a computational model of their biological system.
These models are deposited here.

Make Me My Model For You

Change picture

Web page: http://www.isbe.nl

Programme Administrators: Alexey Kolodkin

Funding details:

No funding details specified

Storage Usage

skype

Venkata Satagopam
is online

5 CORBEL supported services

VIP: Margarida D. Amaral - Cystic Fibrosis Transmembrane Regulator maturation

Anna Maria Colangelo - Modelling ROS management and mitochondrial dysfunction in models of Parkinson disease
VID: 3441 - Molecular Cell Physiology, Vrije University Amsterdam Awaiting Conrmation | Fitting the dynamic model to experimental data
CORBEL Track 2VID: 3444 - Chemogenomics (ChEMBL) at EMBL/EBI Awaiting Confirmation | Profiling of chemotypes for potential off-target effects, measured ADMET properties, in-vivo efcacies
CORBEL Track 2VID: 3447 - Advanced Light Microscopy Facility at EMBL Awaiting Conrmation | Fluorescence resonance energy transfer (FRET) - EMBL HDAwaiting Conrmation | Electron microsocpy - EMBL HD

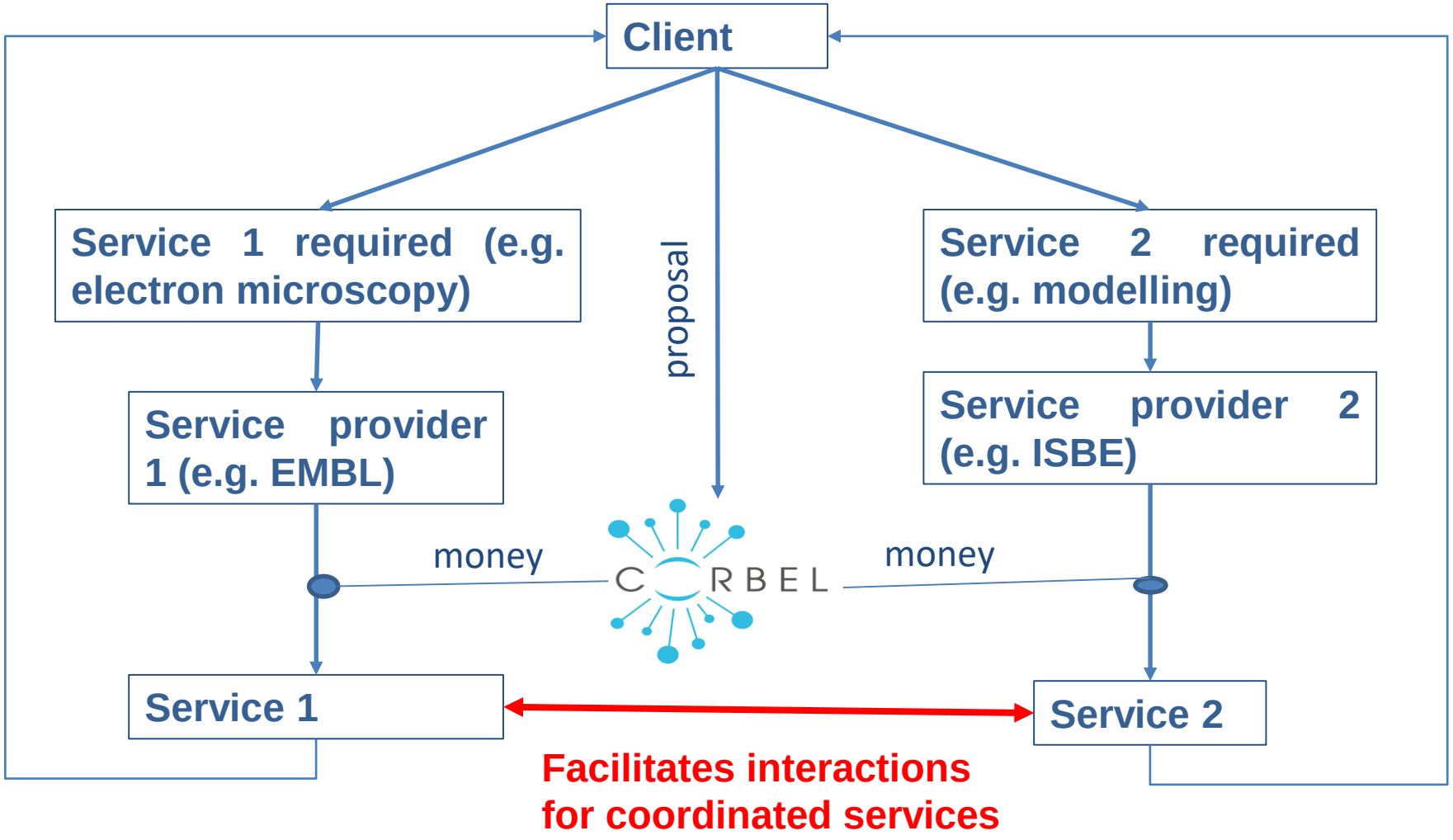
Vikas Kumar EDC-SysTox: Approaches towards Systems Toxicology model via coupled PBPK/PD-system biology benchmarking dosimetry for safety assessment of Endocrine Disrupting Chemical
VID: 3421 - Molecular Cell Physiology, Vrije University Amsterdam
CORBEL Track 2VID: 3422 - Chemogenomics (ChEMBL) at EMBL/EBI
CORBEL Track 2VID: 3423 - Screening and medicinal chemistry at Leibniz-Institute for Molecular Pharmacology (FMP)

Veronika Stoka Jožef Stefan Institute (Slovenia) - Protease signaling network in neurodegeneration

With Chemogenomics (ChEMBL) at EMBL/EBI; Advanced Light Microscopy Facility at EMBL; - Screening and medicinal chemistry at Leibniz-Institute for Molecular Pharmacology (FMP)

Maria Correia - Molecular Insight into Autism Spectrum Disorder (ASD)
1VID: 3248 - Biological Research Fondation Academy of Athens BRFAA Awaiting Conrmation | Genomics and transcriptomics services
CORBEL Track 1VID: 3530 - Molecular Cell Physiology, Vrije University Amsterda

CORBEL supported services:
Integration of Systems Biological Infrastructures



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Modelling ROS management and mitochondrial dysfunction (Milan)

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Mitochondria produce energy and reactive oxygen species (ROS), but suffer from ROS.

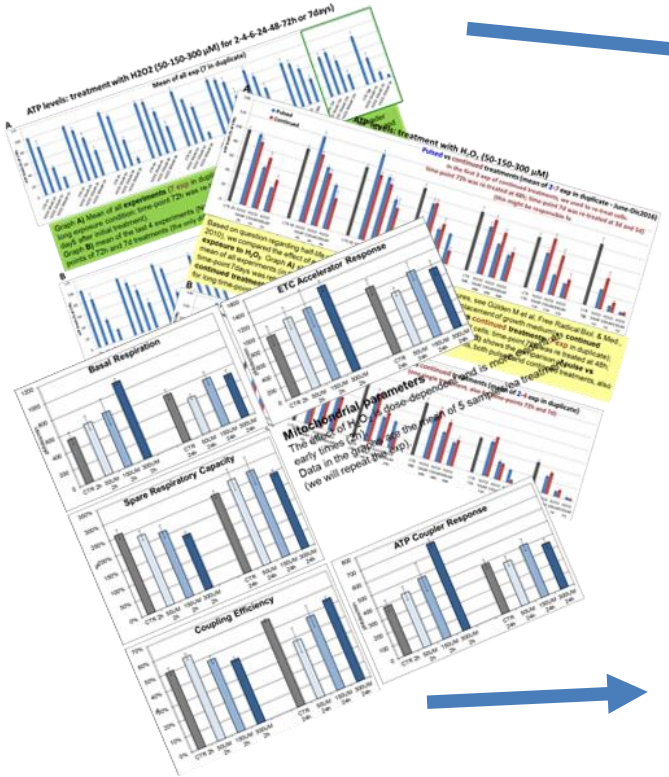
Supported by SYSBIO CENTRE OF SYSTEMS BIOLOGY

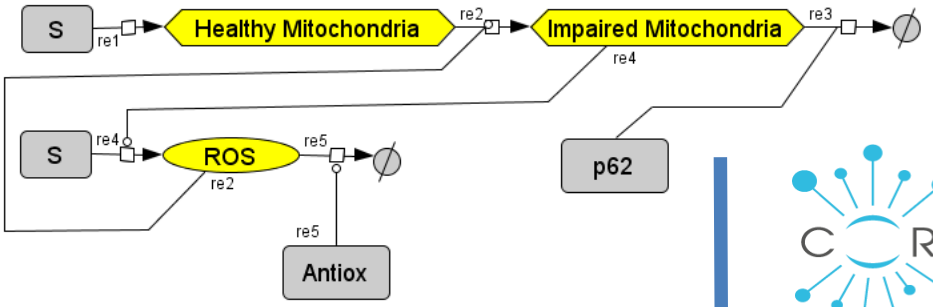
Prof. Lilia Alberghina

Dr. Annamaria Colangelo

Experimental data from University Milan-Bicocca

Experimentally fitted model for understanding mitochondrial dysfunction in Parkinson's disease





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For model validation and application

Advanced Light Microscopy Facility, Fluorescence resonance energy transfer (FRET) at EMBL and Electron microsocpy at EMBL

Profiling of chemotypes for potential off-target effects at Chemogenomics (ChEMBL)

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Safety assessment of endocrine disrupting chemicals (Tarragona, Spain)

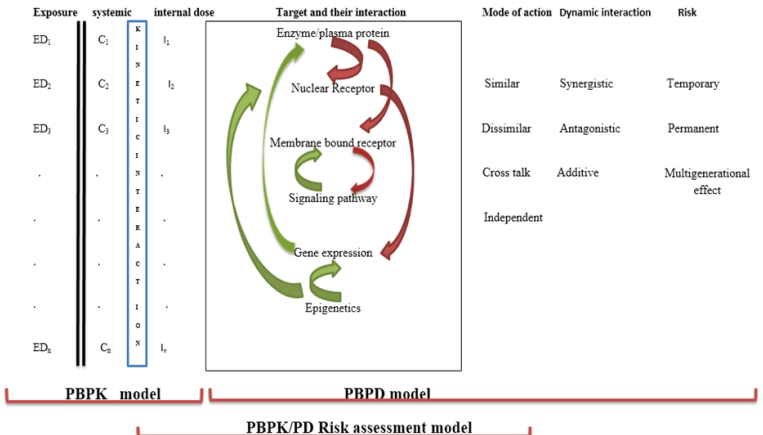
Pesticides, plastics, cosmetics, electrical transformers and many other products contain Endocrine disruptors (EDCs). EDCs interfere with natural hormone functions and may cause the disease.

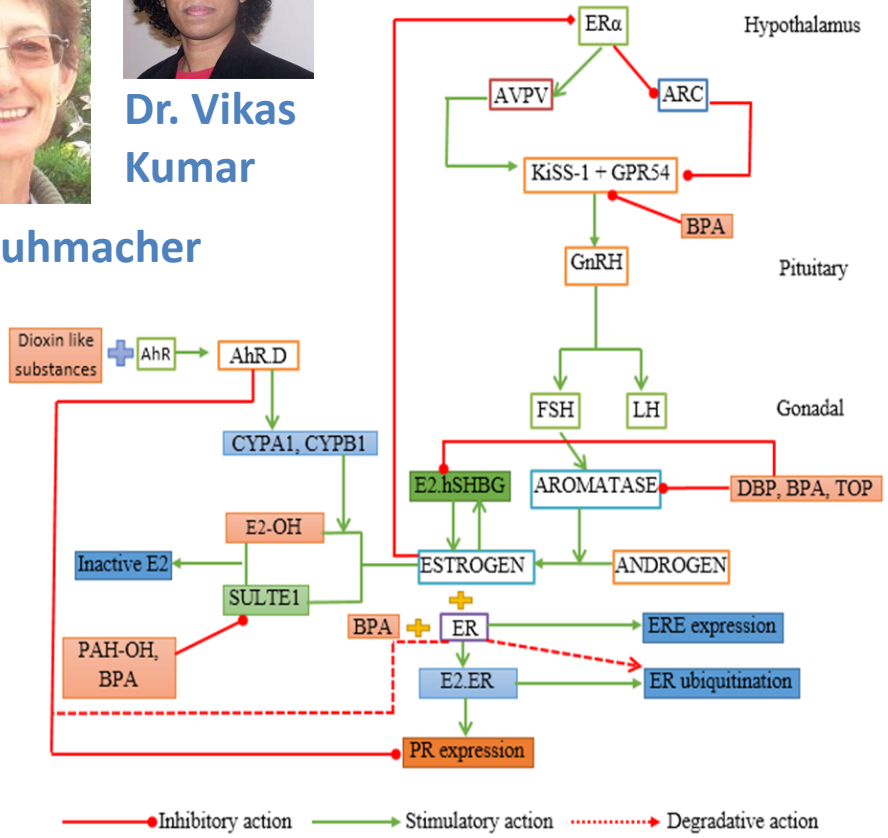
UNIVERSITAT ROVIRA I VIRGILI

Raju Prasad Sharma

Prof. Marta Schuhmacher

Dr. Vikas Kumar





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ROS management in Parkinson's disease and cancer (LCSB, Luxembourg)

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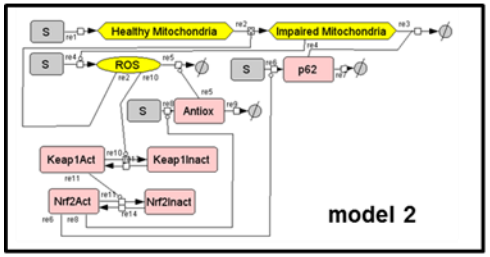
ROS – Reactive Oxygen Species, cause oxidative stress and take part in the disease.

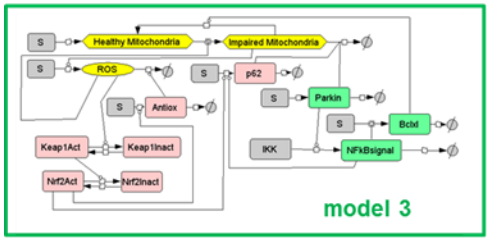
Supported by

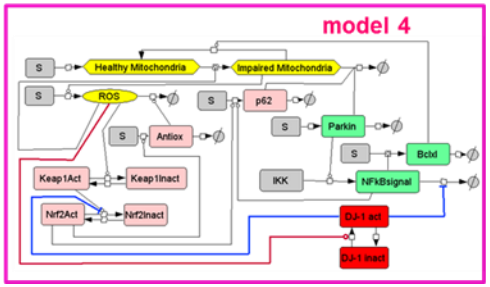
Luxembourg Centre for Systems Biomedicine

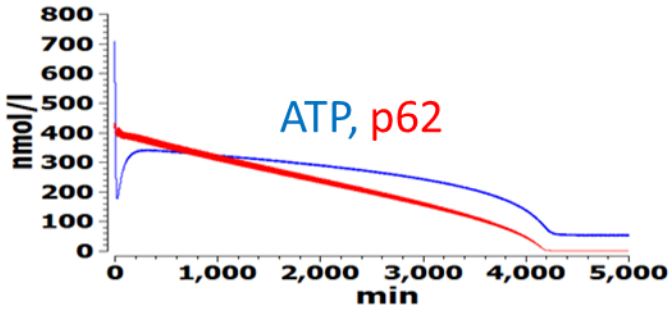
Parkinson's disease

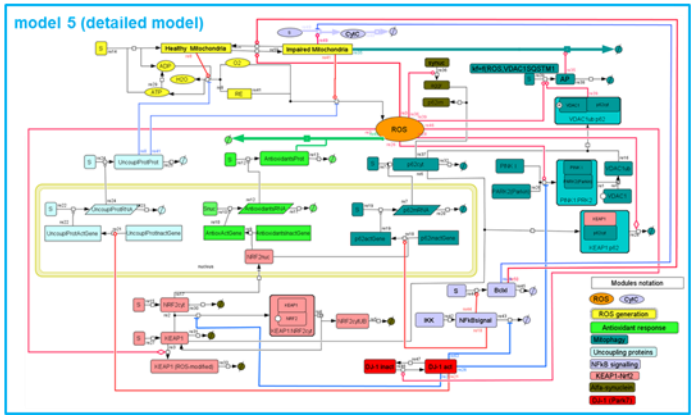
Cancer

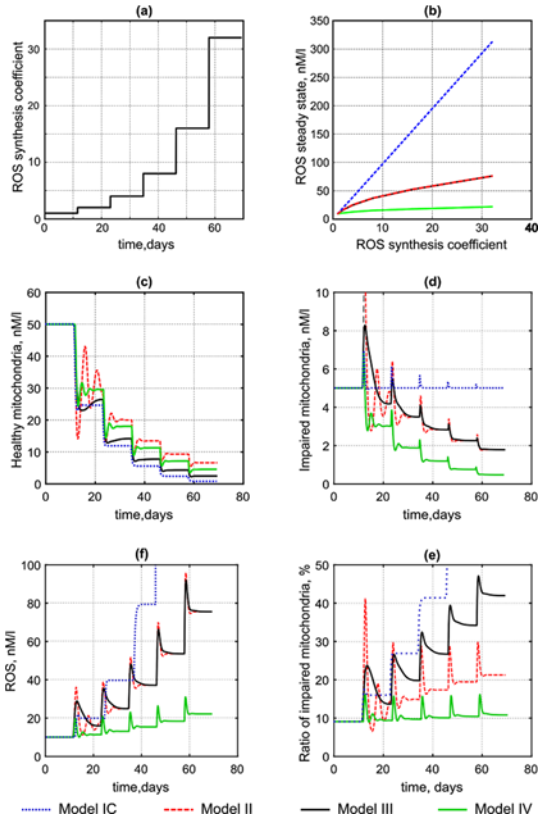












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Mitochondrial perfect adaptation (Sheffield, UK)

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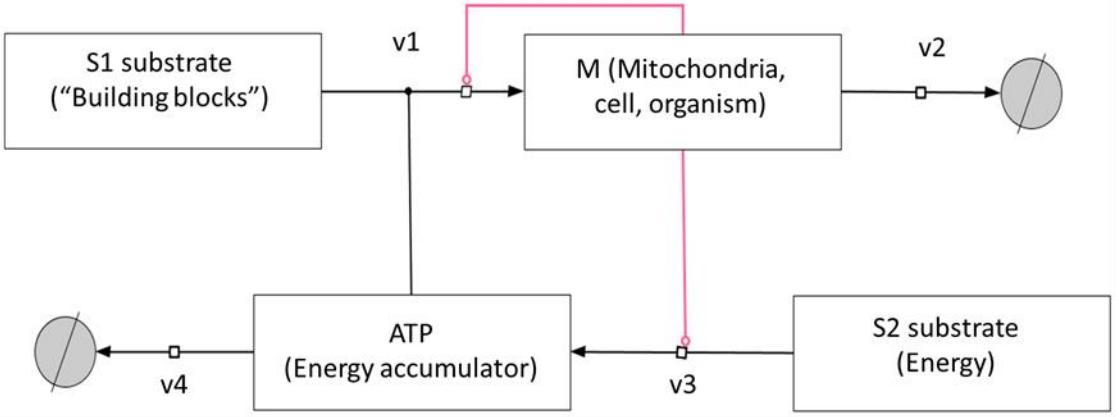
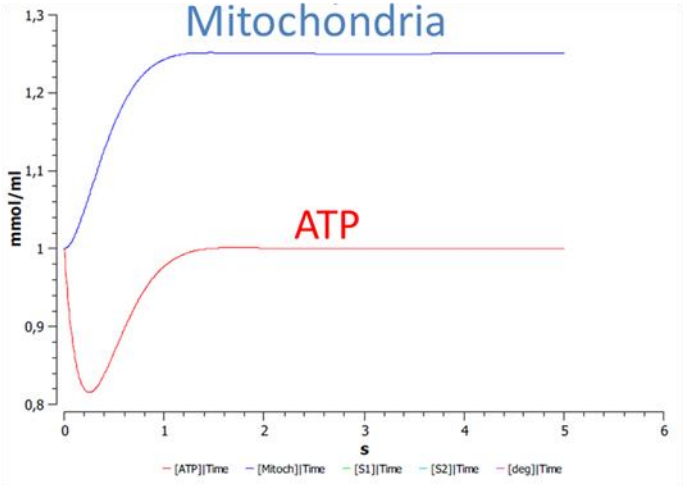
Some processes of biological system are very robust (maintaining ATP level), because other processes are very flexible (mitochondrial activity)

Dr. Fei He





Metabolic Control Analysis Result

Steady State found. All coefficients available.

Elasticities | Flux Control Coefficients | Concentration Control Coefficients

Rows (effect): Species (reduced system)

Columns (cause): Reactions (reduced system)

	(reaction_1)	(reaction_2)	(reaction_3)	(reaction_4)
ATP	1	-1	0	0
Mitoch	1	-0.75	-1.25	1

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CFTR maturation (Lisbon, Portugal)

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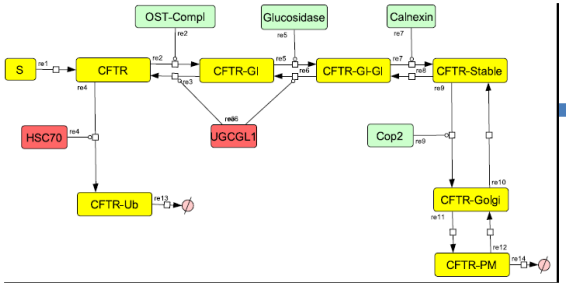
Cystic Fibrosis (CF)- lethal autosomic disease
CFTR - Cystic Fibrosis Transmembrane Regulator

Supported by

CORBEL

Dr. Hugo Botelho

Prof. Margarida D. Amaral



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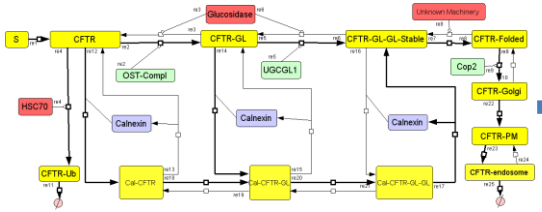

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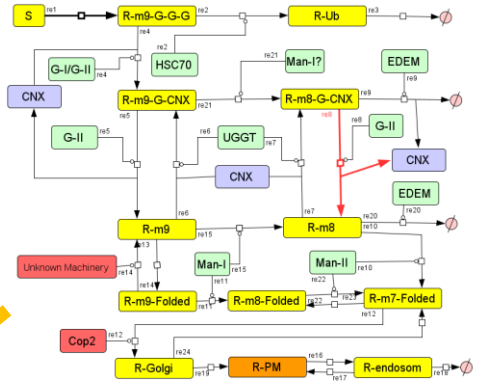

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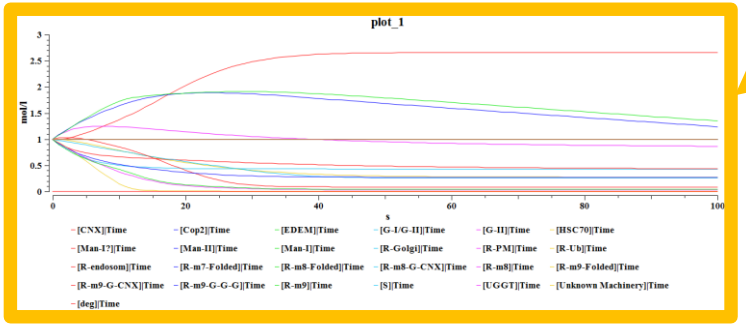

Version 4

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Projects with Essen (Germany): Cool design of Hot metabolism in Archaea

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Prof. Bettina Siebers

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Projects with Essen (Germany): The Yin-Yang of Metabolism; Endometatoxicity (YYME)

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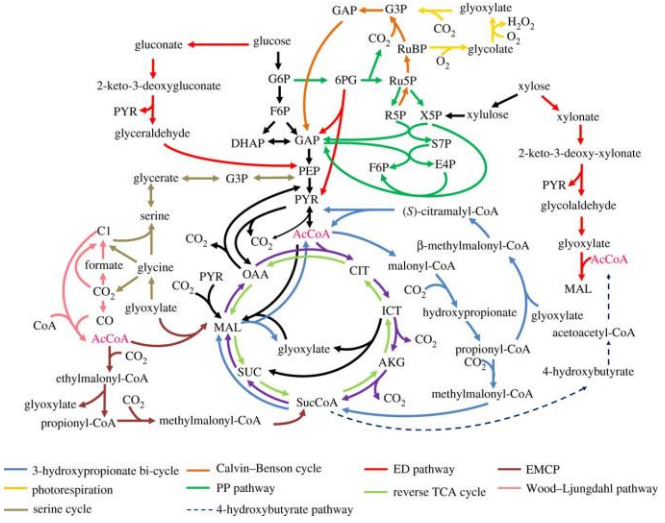
Prof. Bettina Siebers

A shadow side of good metabolism – intracellular production and fortuitous accumulation of toxic chemical compounds.



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Charged peptide to charged membrane binding model (Munich, Germany)

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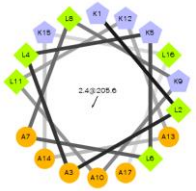
Electric repulsion or attraction should be taken into account to understand membrane-protein interactions.

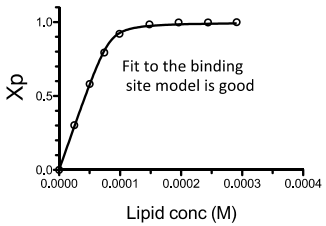
Dr. Frits Kamp

Binding of a positively charged amphipathic helix to a negatively charged membrane

KLAK peptide:
Ac-**C**(Bimane)-
KLALKLALKALKAAKLA

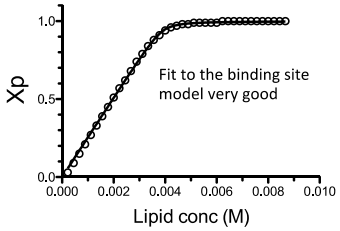


Fluorescence experiment of KLAK (3 μM) binding to Small Unilamellar Vesicles (SUV) containing 10% POPS

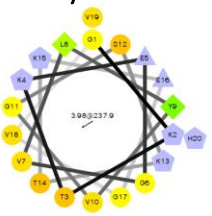


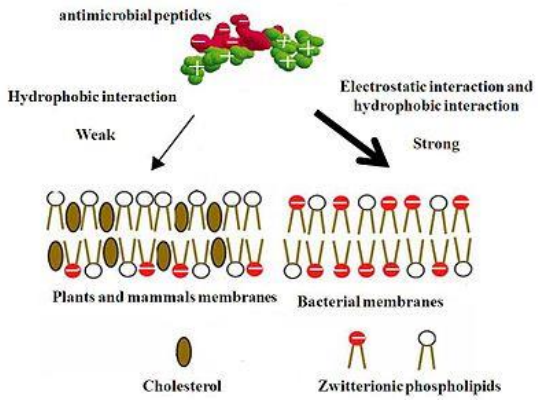
Binding of a positively charged amphipathic helix (with a strongly negatively charged unstructured C-terminus) to a neutral (zwitterionic) membrane

Isothermal Titration Calorimetry experiment of α-syn (9 μM) binding to SUV DPPC



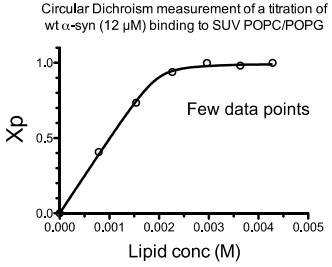
α-synuclein





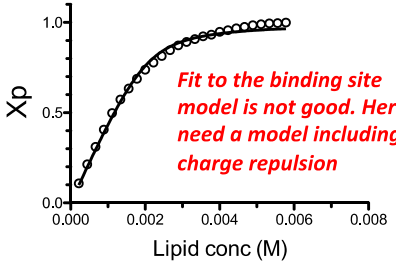
Binding of a positively charged amphipathic helix (with a strongly negatively charged unstructured C-terminus) to a negatively charged membrane

Circular Dichroism measurement of a titration of wt α-syn (12 μM) binding to SUV POPC/POPG



Binding of a positively charged amphipathic helix (with a strongly negatively charged unstructured C-terminus) to a negatively charged membrane

ITC experiment of α−syn (9 μM) binding to SUV POPC/POPG



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Modelling substrate diffusion and metabolism in biofilms (Helmholtz Center Munich, Germany)

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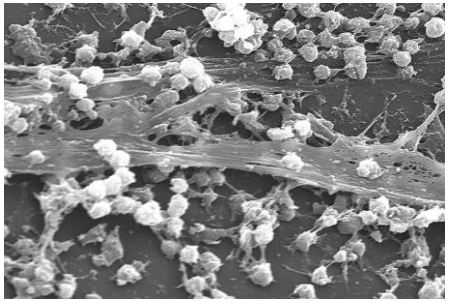
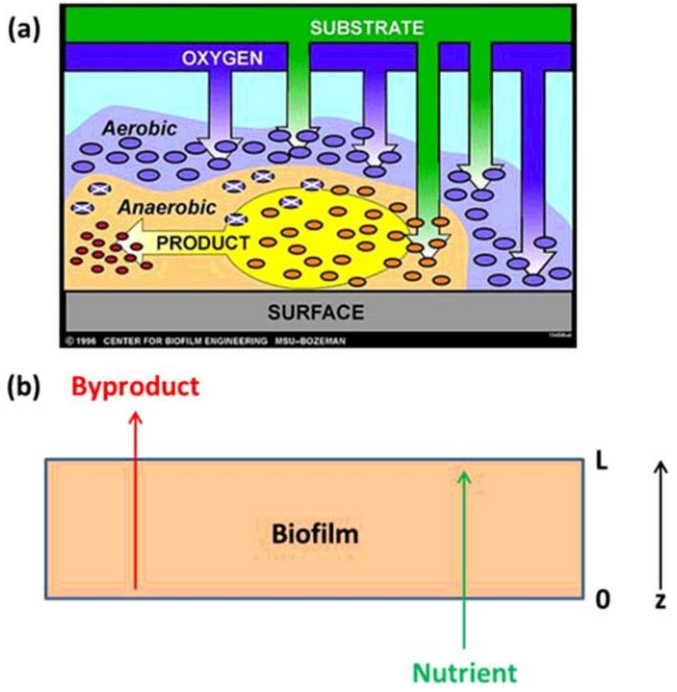
A biofilm is any group of microorganisms in which cells stick to each other and often these cells adhere to a surface. This affects the diffusion of substrates to cells and their metabolsim.

Dr. Martin Elsner





Thank you!