Bundesinstitut für Risikobewertung

FEDERAL INSTITUTE
FOR RISK ASSESSMENT

Available Community Tools for Predictive Modelling

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Outline

Overview on currently available community resources

Introduction to PMM-Lab software

Introduction to openFSMR model repository

Community resources Predictive Modelling

Microbial growth, survival, inactivation **data**:

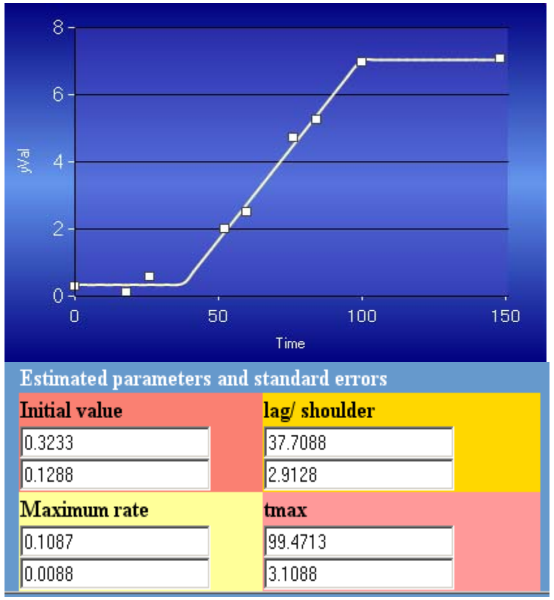
Scientific publications

ComBase http://www.combase.cc

Sym’Previus http://www.symprevius.org (subscription)

Currently available Predictive Modelling

Tools for **model generation**:



Estimated parameters and standard errors

Initial value	lag/ shoulder
0.3233	37.7088
0.1288	2.9128

Maximum rate	tmax
0.1087	99.4713
0.0088	3.1088

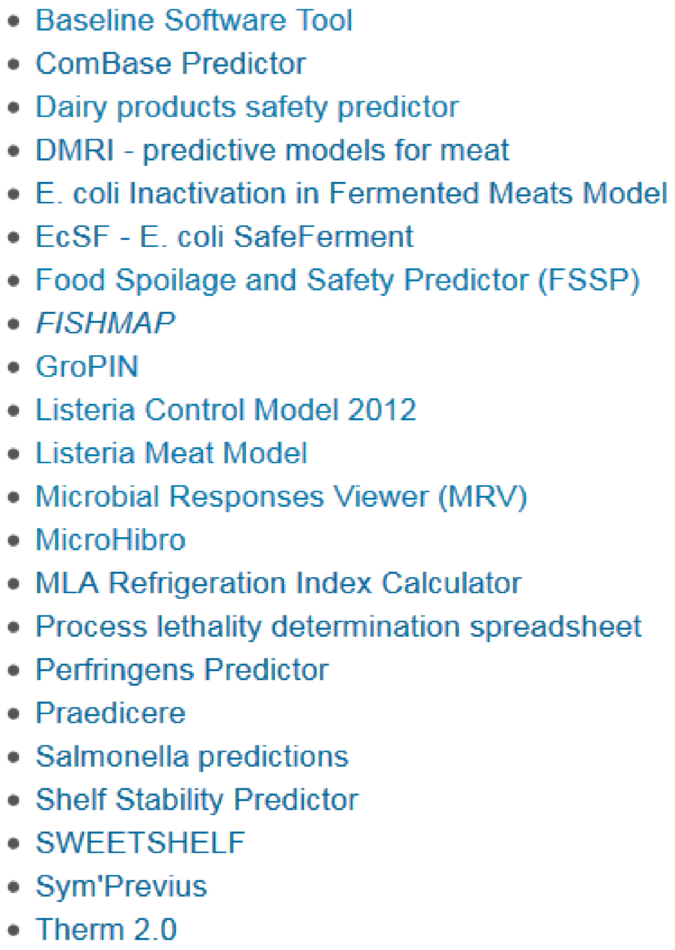
$$y(t) = y_o + \mu_{\max} A(t) - \frac{1}{m} \ln\left(1 + \frac{\exp(m\mu_{\max} A(t)) - 1}{\exp(m(y_{\max} - y_o))}\right)$$

$$A(t) = t + \frac{1}{v} \ln\left(\frac{\exp(-vt) + q_o}{1 + q_o}\right)$$

DMFit	**www.ifr.ac.uk/safety/dmfit/**
GInaFiT	**http://cit.kuleuven.be/biotec/downloads.php**
IPMP	**www.ars.usda.gov/Services/Docs.htm?docid=23355**
nlsMicrobio (R)	**https://cran.r-project.org/web/packages/nlsMicrobio/index.html**
PMM-Lab	**https://sourceforge.net/projects/pmmlab**
OptiPa	**www.optipa.be**

Currently available community resources in the area of Predictive Modelling

Tools for **model-based predictions**


- Baseline Software Tool
- ComBase Predictor
- Dairy products safety predictor
- DMRI - predictive models for meat
- E. coli Inactivation in Fermented Meats Model
- EcSF - E. coli SafeFerment
- Food Spoilage and Safety Predictor (FSSP)
- *FISHMAP*
- GroPIN
- Listeria Control Model 2012
- Listeria Meat Model
- Microbial Responses Viewer (MRV)
- MicroHibro
- MLA Refrigeration Index Calculator
- Process lethality determination spreadsheet
- Perfringens Predictor
- Praedicere
- Salmonella predictions
- Shelf Stability Predictor
- SWEETSHELF
- Sym'Previus
- Therm 2.0

https://sourceforge.net/p/microbialmodelingexchange/wiki/Tools/

Search engine and Repository of predictive models:

openFSMR

Created by BfR and UD

Summary

=> Plenty of data and predictive microbial models available or published in scientific literature

=> Several software tools for model-based predictions available

(GroPIN, PMP, FSSP, Sym'Previus, MRV, ComBase Predictor …)

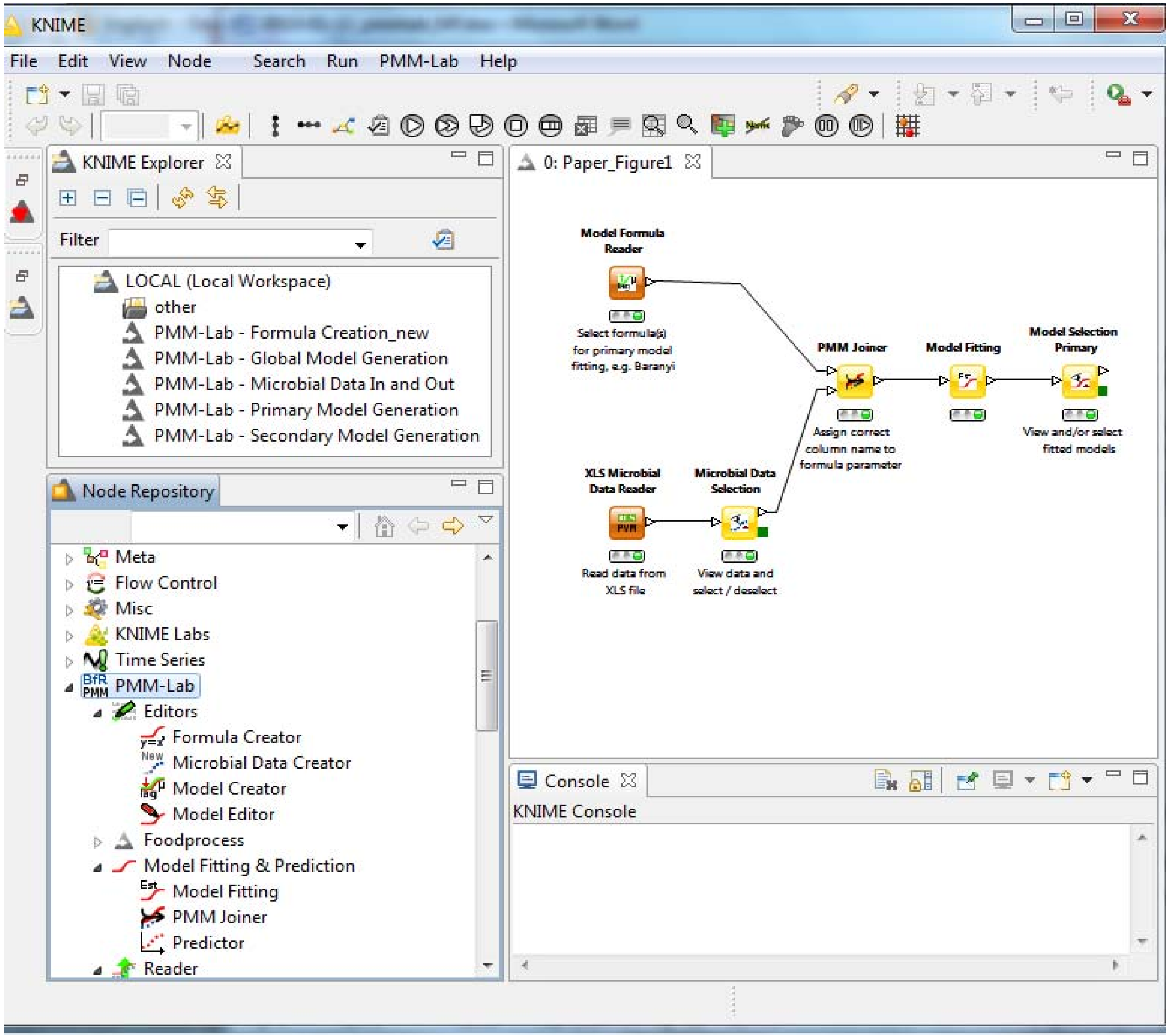
Current challenges:

- Integrated data management process from data to models
- Annotation of data and models (e.g. nomenclature of food matrices)
- Frequently: reimplementation of models needed
- No "information exchange" between available tools

WHY:

- NO harmonized file format for exchange of data / models
- FEW open-source software solutions
- Too many "island solutions"

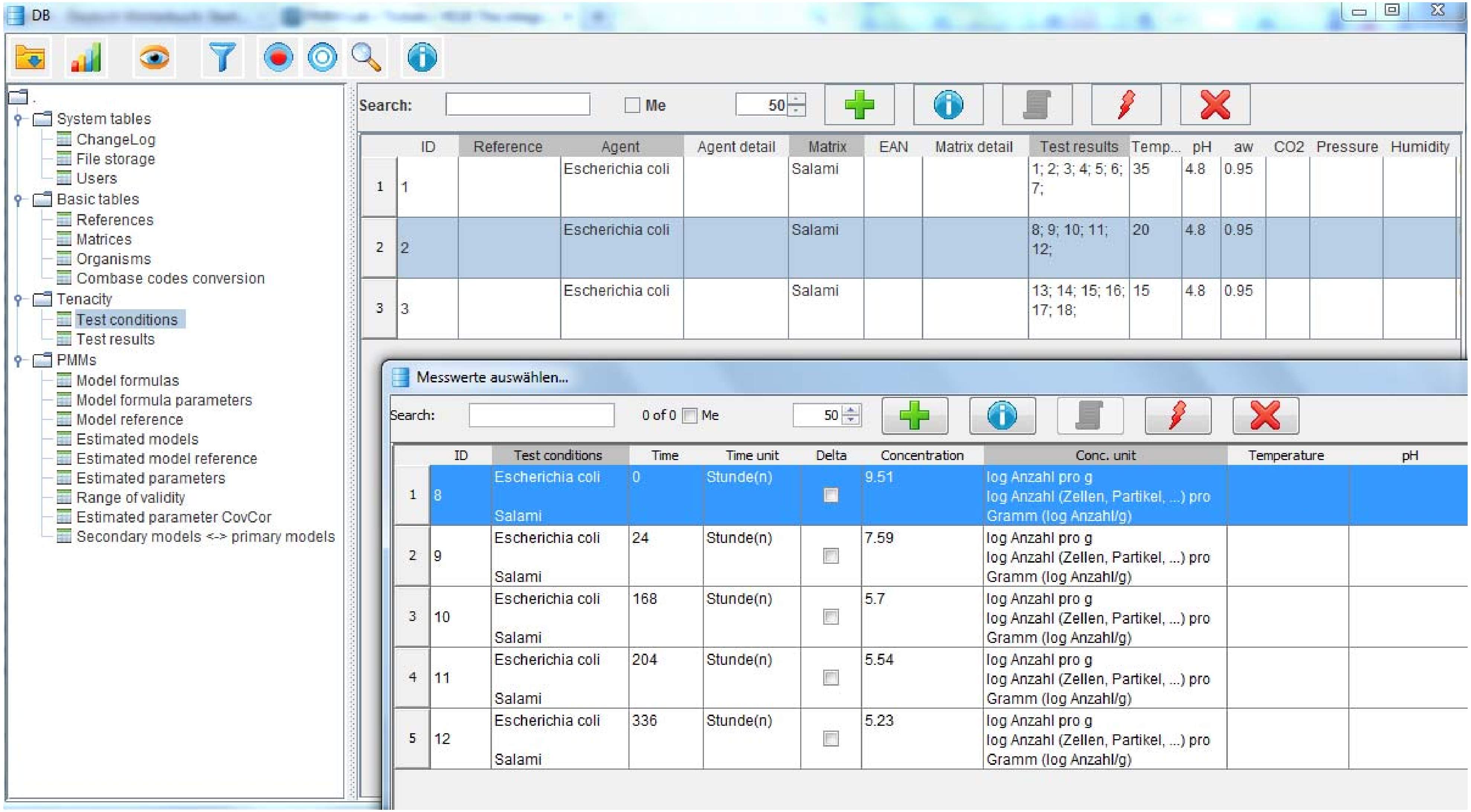
PMM-Lab
“Predictive Microbial Modelling – Lab”



„Graphical programming“
microbial modelling tool

extending the
KNIME
open source
data analytics platform

PMM-Lab – Features
“Integrated pre-configured database”



- System tables
  - ChangeLog
  - File storage
  - Users
- Basic tables
  - References
  - Matrices
  - Organisms
  - Combase codes conversion
- Tenacity
  - Test conditions
  - Test results
- PMMs
  - Model formulas
  - Model formula parameters
  - Model reference
  - Estimated models
  - Estimated model reference
  - Estimated parameters
  - Range of validity
  - Estimated parameter CovCor
  - Secondary models <-> primary models

Search: ☐ Me 50

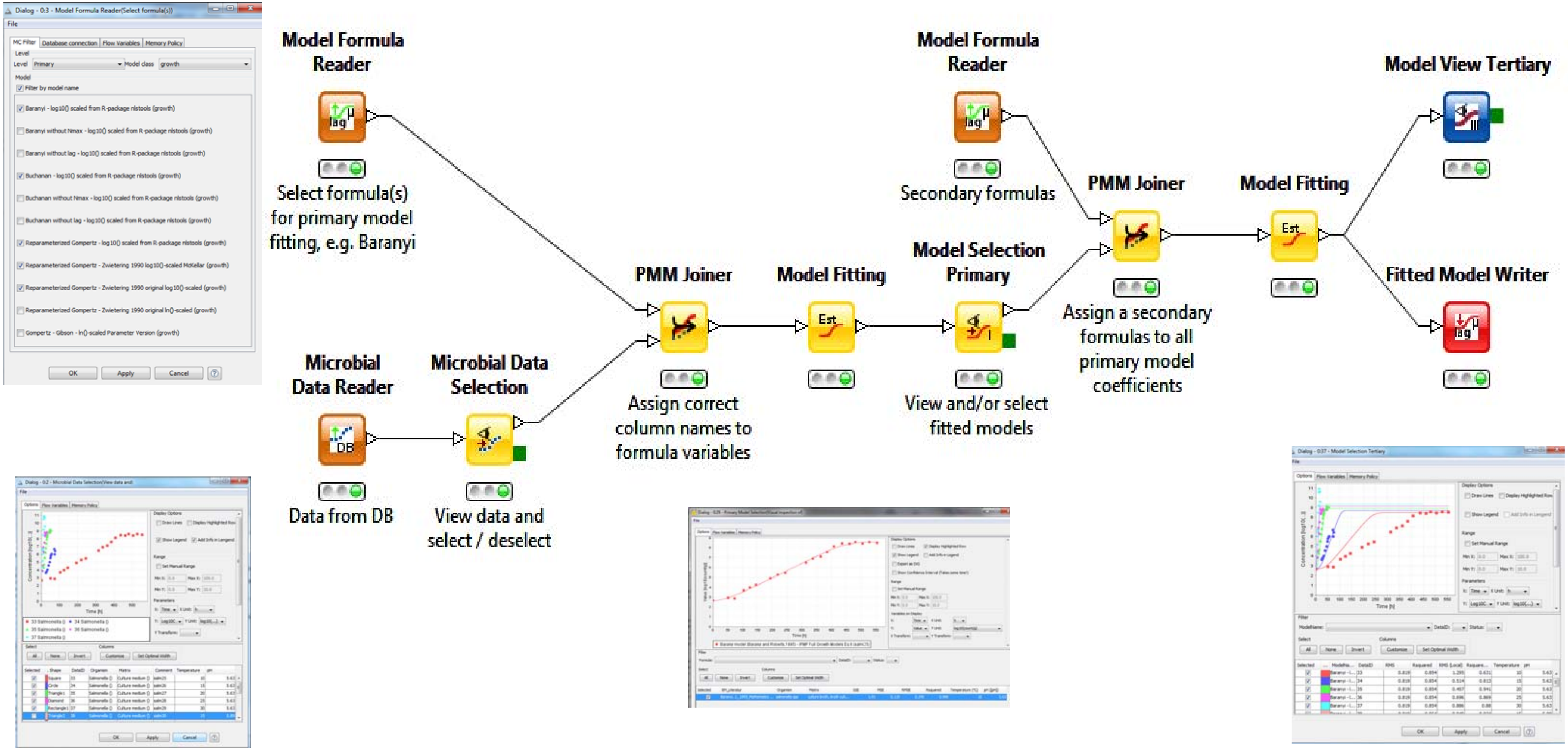
	ID	Reference	Agent	Agent detail	Matrix	EAN	Matrix detail	Test results	Temp...	pH	aw	CO2	Pressure	Humidity
1	1		Escherichia coli		Salami			1; 2; 3; 4; 5; 6; 7;	35	4.8	0.95			
2	2		Escherichia coli		Salami			8; 9; 10; 11; 12;	20	4.8	0.95			
3	3		Escherichia coli		Salami			13; 14; 15; 16; 17; 18;	15	4.8	0.95			

Messwerte auswählen...

Search: 0 of 0 ☐ Me 50

	ID	Test conditions	Time	Time unit	Delta	Concentration	Conc. unit	Temperature	pH
1	8	Escherichia coli Salami	0	Stunde(n)	☐	9.51	log Anzahl pro g log Anzahl (Zellen, Partikel, ...) pro Gramm (log Anzahl/g)		
2	9	Escherichia coli Salami	24	Stunde(n)	☐	7.59	log Anzahl pro g log Anzahl (Zellen, Partikel, ...) pro Gramm (log Anzahl/g)		
3	10	Escherichia coli Salami	168	Stunde(n)	☐	5.7	log Anzahl pro g log Anzahl (Zellen, Partikel, ...) pro Gramm (log Anzahl/g)		
4	11	Escherichia coli Salami	204	Stunde(n)	☐	5.54	log Anzahl pro g log Anzahl (Zellen, Partikel, ...) pro Gramm (log Anzahl/g)		
5	12	Escherichia coli Salami	336	Stunde(n)	☐	5.23	log Anzahl pro g log Anzahl (Zellen, Partikel, ...) pro Gramm (log Anzahl/g)		

PMM-Lab – Features
“Model generation and statistics”



Dialog - 0:3 - Model Formula Reader(Select formula(s))

Level
Level: Primary
Model class: growth

Model
☑ Filter by model name

☑ Baranyi - log10() scaled from R-package nlstools (growth)
☐ Baranyi without Nmax - log10() scaled from R-package nlstools (growth)
☐ Baranyi without lag - log10() scaled from R-package nlstools (growth)
☑ Buchanan - log10() scaled from R-package nlstools (growth)
☐ Buchanan without Nmax - log10() scaled from R-package nlstools (growth)
☐ Buchanan without lag - log10() scaled from R-package nlstools (growth)
☑ Reparameterized Gompertz - log10() scaled from R-package nlstools (growth)
☑ Reparameterized Gompertz - Zwietering 1990 log10()-scaled McKellar (growth)
☑ Reparameterized Gompertz - Zwietering 1990 original log10()-scaled (growth)
☐ Reparameterized Gompertz - Zwietering 1990 original ln()-scaled (growth)
☐ Gompertz - Gibson - ln()-scaled Parameter Version (growth)

Model Formula Reader

Select formula(s) for primary model fitting, e.g. Baranyi

Microbial Data Reader

Data from DB

Microbial Data Selection

View data and select / deselect

PMM Joiner

Assign correct column names to formula variables

Model Fitting

Model Selection Primary

View and/or select fitted models

Model Formula Reader

Secondary formulas

PMM Joiner

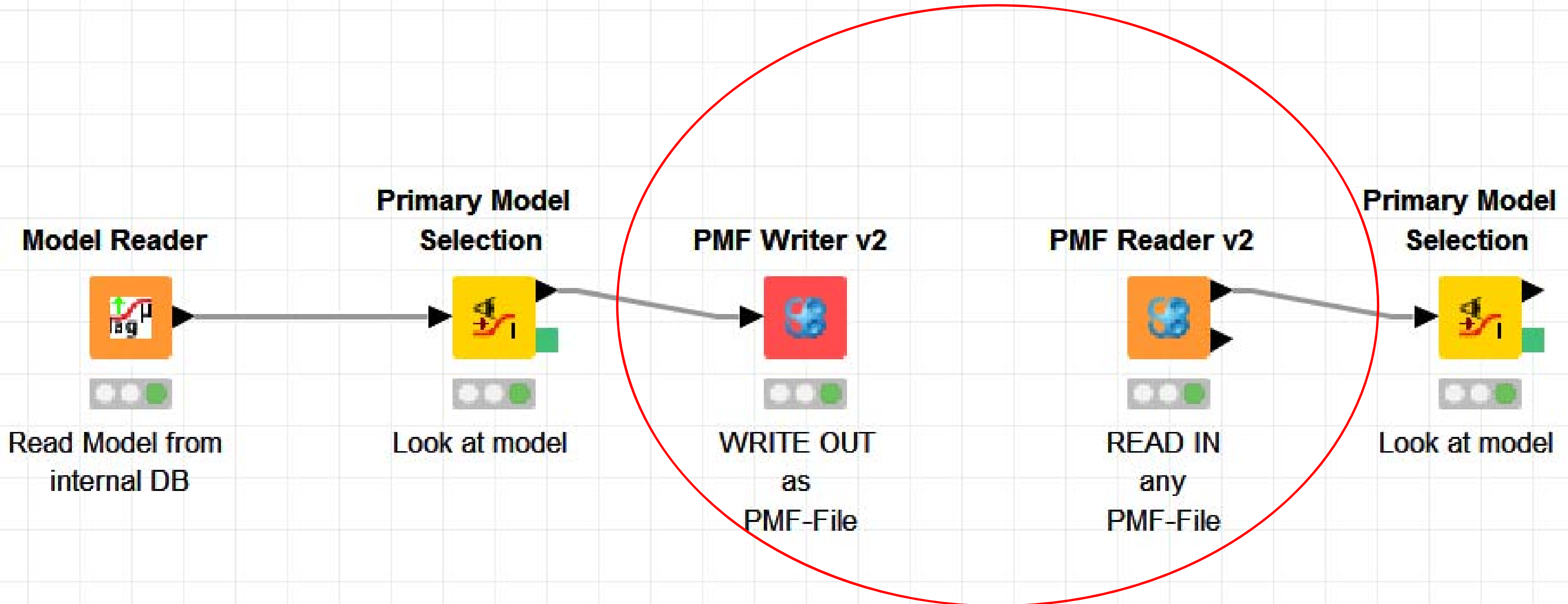
Assign a secondary formulas to all primary model coefficients

Model Fitting

Model View Tertiary

Fitted Model Writer

PMM-Lab – Features
“Model Import / Export”



Model Reader

Read Model from internal DB

Primary Model Selection

Look at model

PMF Writer v2

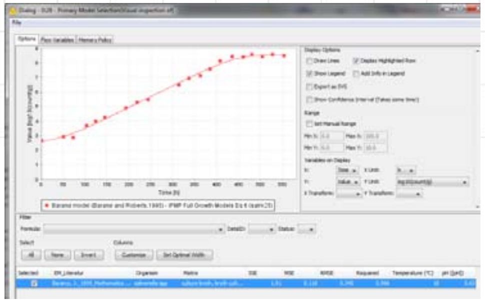
WRITE OUT as PMF-File

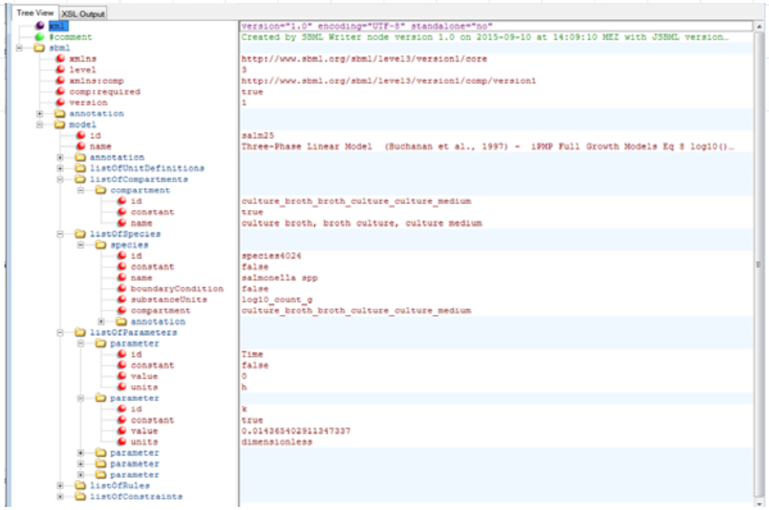
PMF Reader v2

READ IN any PMF-File

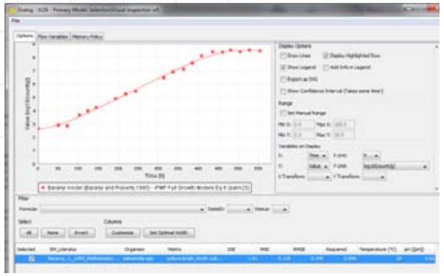
Primary Model Selection

Look at model

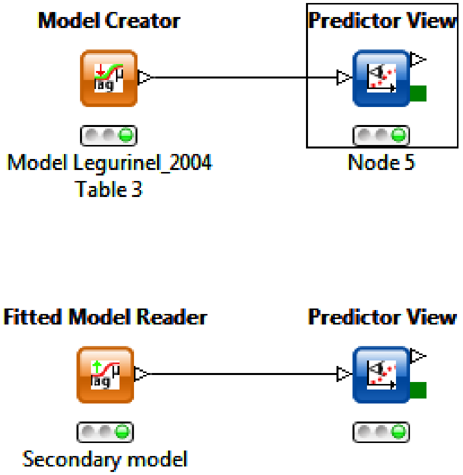


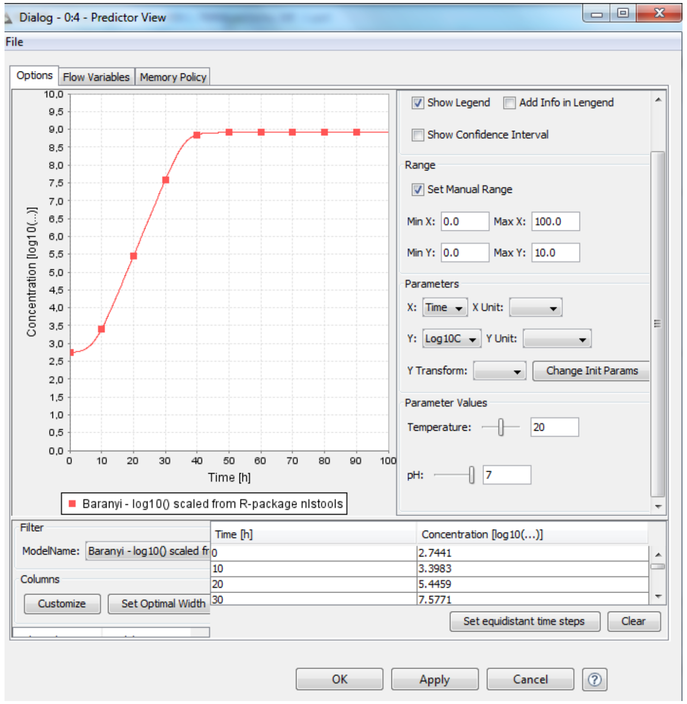


```
xml                                version="1.0" encoding="UTF-8" standalone="no"
#comment                           Created by SBML Writer node version 1.0 on 2015-09-10 at 14:09:10 MEZ with JSBML version…
sbml
  xmlns                            http://www.sbml.org/sbml/level3/version1/core
  level                            3
  xmlns:comp                       http://www.sbml.org/sbml/level3/version1/comp/version1
  comp:required                    true
  version                          1
  annotation
  model
    id                             salm25
    name                           Three-Phase Linear Model  (Buchanan et al., 1997) -  1PMP Full Growth Models Eq 8 log10()…
    annotation
    listOfUnitDefinitions
    listOfCompartments
      compartment
        id                         culture_broth_broth_culture_culture_medium
        constant                   true
        name                       culture broth, broth culture, culture medium
    listOfSpecies
      species
        id                         species4024
        constant                   false
        name                       salmonella spp
        boundaryCondition          false
        substanceUnits             log10_count_g
        compartment                culture_broth_broth_culture_culture_medium
        annotation
    listOfParameters
      parameter
        id                         Time
        constant                   false
        value                      0
        units                      h
      parameter
        id                         k
        constant                   true
        value                      0.014365402911347337
        units                      dimensionless
      parameter
      parameter
      parameter
    listOfRules
    listOfConstraints
```



PMM-Lab – Features
“Generic model-based predictions”





☑ Show Legend ☐ Add Info in Lengend

☐ Show Confidence Interval

Range

☑ Set Manual Range

Min X: 0.0 Max X: 100.0

Min Y: 0.0 Max Y: 10.0

Parameters

X: Time X Unit:

Y: Log10C Y Unit:

Parameter Values

Temperature: 20

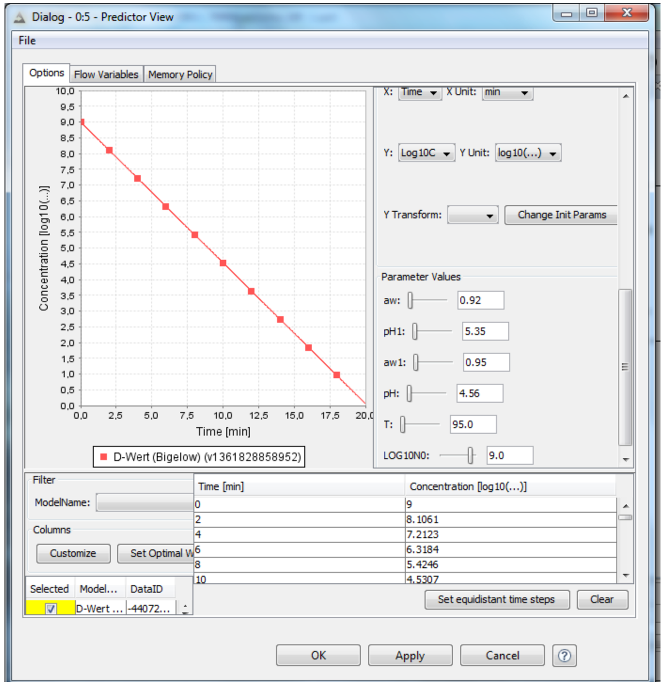
pH: 7

🟥 Baranyi - log10() scaled from R-package nlstools

Filter

ModelName: Baranyi - log10() scaled fr

Time [h]	Concentration [log10(...)]
0	2.7441
10	3.3983
20	5.4459
30	7.5771



X: Time X Unit: min

Y: Log10C Y Unit: log10(...)

Y Transform:

Parameter Values

aw: 0.92

pH1: 5.35

aw1: 0.95

pH: 4.56

T: 95.0

LOG10N0: 9.0

🟥 D-Wert (Bigelow) (v1361828858952)

Filter

ModelName:

Selected	Model...	DataID
☑	D-Wert ...	-44072...

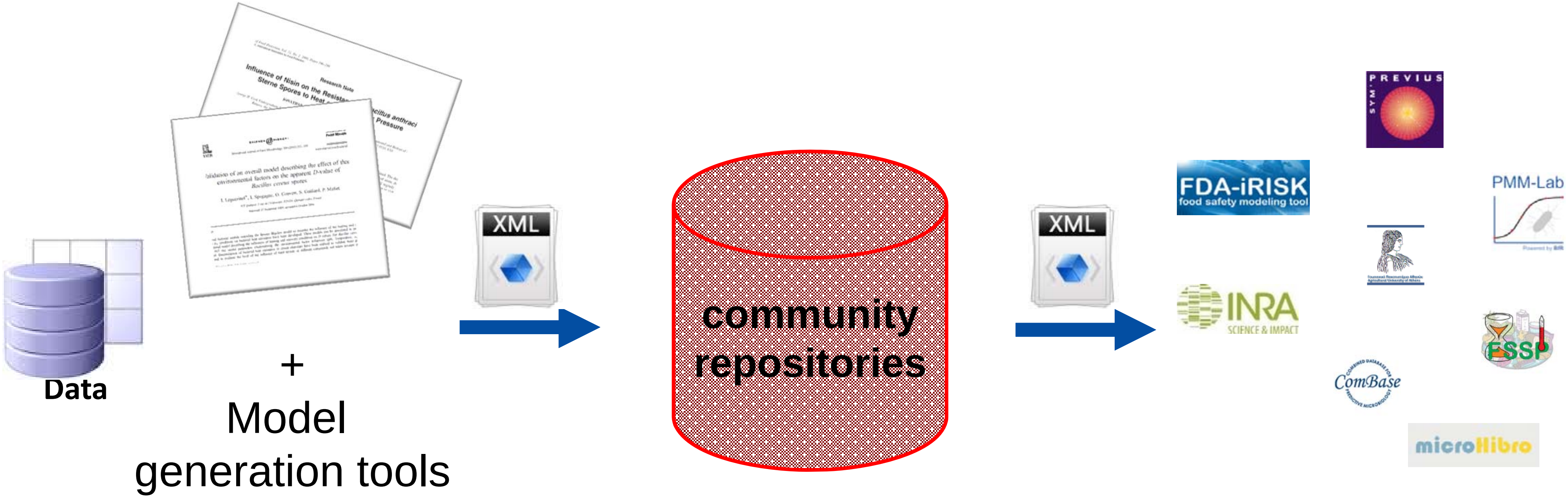
Time [min]	Concentration [log10(...)]
0	9
2	8.1061
4	7.2123
6	6.3184
8	5.4246
10	4.5307

Advantages of the PMM-Lab framework

- Free, open-source, transparent
- Data management integrated (raw data, model generation process, estimated models)
- Modular, highly flexible, easy-to-extend, easy-to-reuse
- Integrated into KNIME (provides integration of „R“, MATLAB, Data mining, Report generation etc.)
- Infrastructure for community contributions available: Code repository, Wiki, File download (e.g.sample files), Ticket system
- Exchange of workflows and models -> sharing of knowledge with others

BfR-Vision

Community-driven, curated repositories of microbial models (Food Safety Knowledge Bases)



Data

+
Model
generation tools

community repositories

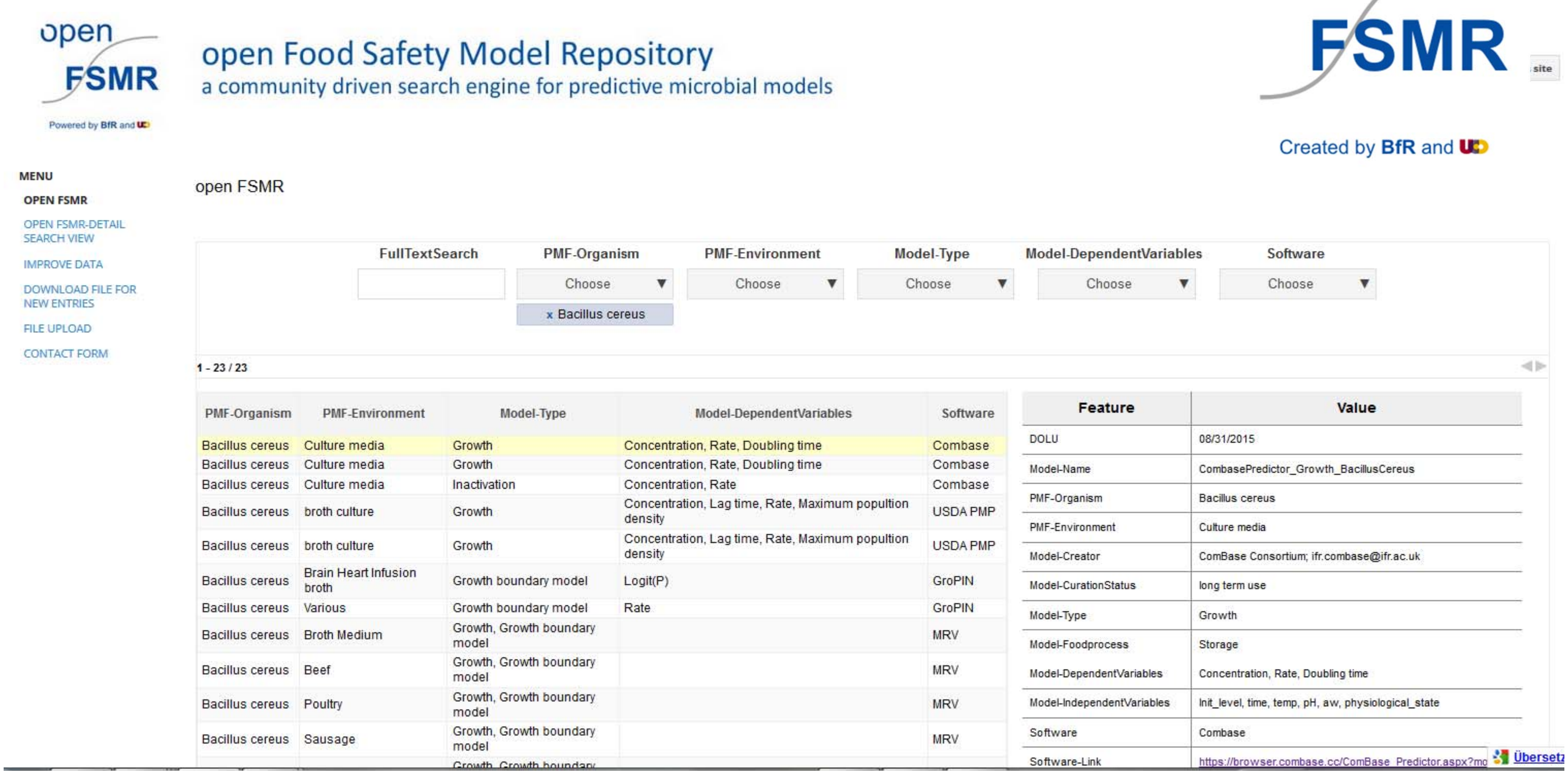
Newly generated models / re-implemented models

Model Repository with GUI to search and model download

Model deployment

openFSMR

Created by BfR and UD



PMF-Organism	PMF-Environment	Model-Type	Model-DependentVariables	Software
Bacillus cereus	Culture media	Growth	Concentration, Rate, Doubling time	Combase
Bacillus cereus	Culture media	Growth	Concentration, Rate, Doubling time	Combase
Bacillus cereus	Culture media	Inactivation	Concentration, Rate	Combase
Bacillus cereus	broth culture	Growth	Concentration, Lag time, Rate, Maximum popultion density	USDA PMP
Bacillus cereus	broth culture	Growth	Concentration, Lag time, Rate, Maximum popultion density	USDA PMP
Bacillus cereus	Brain Heart Infusion broth	Growth boundary model	Logit(P)	GroPIN
Bacillus cereus	Various	Growth boundary model	Rate	GroPIN
Bacillus cereus	Broth Medium	Growth, Growth boundary model		MRV
Bacillus cereus	Beef	Growth, Growth boundary model		MRV
Bacillus cereus	Poultry	Growth, Growth boundary model		MRV
Bacillus cereus	Sausage	Growth, Growth boundary model		MRV

Feature	Value
DOLU	08/31/2015
Model-Name	CombasePredictor_Growth_BacillusCereus
PMF-Organism	Bacillus cereus
PMF-Environment	Culture media
Model-Creator	ComBase Consortium; ifr.combase@ifr.ac.uk
Model-CurationStatus	long term use
Model-Type	Growth
Model-Foodprocess	Storage
Model-DependentVariables	Concentration, Rate, Doubling time
Model-IndependentVariables	Init_level, time, temp, pH, aw, physiological_state
Software	Combase
Software-Link	https://browser.combase.cc/ComBase_Predictor.aspx?mo

Selected features:

1. Search and filter models (e.g. Organism, Software etc.)
2. Download of models (if provided)
3. Extended model meta-data visible (right pane)

https://sites.google.com/site/openfsmr/

Thanks to the BfR team

Miguel de Alba Aparicio, Armin Weiser, Christian Thöns, Alexander Falenski, Taras Günther, Lars Valentin, Guido Correia Carreira, Carolina Plaza-Rodriguez, Annemarie Käsbohrer, Bernd Appel

Thank you for your attention

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