

bioremediation and the cracked crystal ball

Stephan Richter - Higrade DocConference

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HELMHOLTZ
CENTRE FOR
ENVIRONMENTAL
RESEARCH - UFZ

overview

motivation

toolbox development

database investigation

next steps

motivation

toolbox development

database investigation

next steps



overview

motivation

situation

idea: facilitation of
BIOREMEDIATION
using MULTIPLE
BACTERIAL SPECIES

idea: What are we
aiming for?

toolbox development

database investigation

next steps

motivation



overview

motivation

situation

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BIOREMEDIATION
using MULTIPLE
BACTERIAL SPECIES

idea: What are we
aiming for?

toolbox development

database investigation

next steps

- many former industrial sites



overview

motivation

situation

idea: facilitation of
BIOREMEDIATION
using MULTIPLE
BACTERIAL SPECIES

idea: What are we
aiming for?

toolbox development

database investigation

next steps

- many former industrial sites
- **toxic pollutants** seep into the soil for years/decades



Bundesarchiv, B 146 Bild-F078970-0028
Foto: o. Ang. | Juni 1988

overview

motivation

situation

idea: facilitation of
BIOREMEDIATION
using MULTIPLE
BACTERIAL SPECIES

idea: What are we
aiming for?

toolbox development

database investigation

next steps

- many former industrial sites
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- substances still there, **resist** degradation

overview

motivation

situation

idea: facilitation of
BIOREMEDIATION
using MULTIPLE
BACTERIAL SPECIES

idea: What are we
aiming for?

toolbox development

database investigation

next steps

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- substances still there, **resist** degradation
- for some substances: degraders known

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overview

motivation

situation

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BIOREMEDIATION
using MULTIPLE
BACTERIAL SPECIES

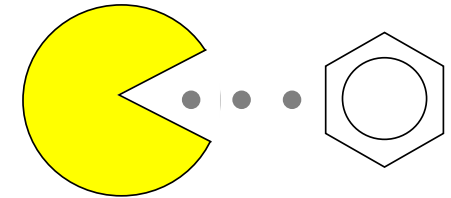
idea: What are we
aiming for?

toolbox development

database investigation

next steps

- potential **degrading bacteria** known
(at least for some contaminants)



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overview

motivation

situation

idea: facilitation of
BIOREMEDIATION
using MULTIPLE
BACTERIAL SPECIES

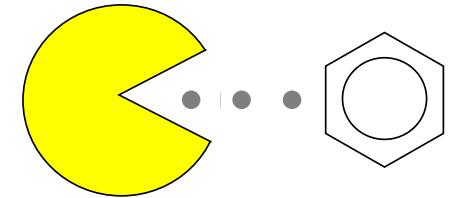
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aiming for?

toolbox development

database investigation

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- how can we take advantage of those bacteria?



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overview

motivation

situation

idea: facilitation of
BIOREMEDIATION
using MULTIPLE
BACTERIAL SPECIES

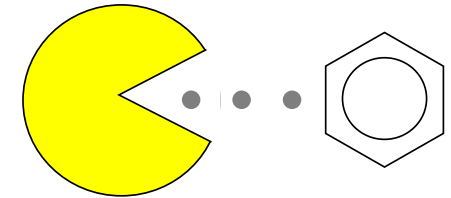
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aiming for?

toolbox development

database investigation

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- can't we use them for **facilitation of contaminat removal**?



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overview

motivation

situation

idea: facilitation of
BIOREMEDIATION
using MULTIPLE
BACTERIAL SPECIES

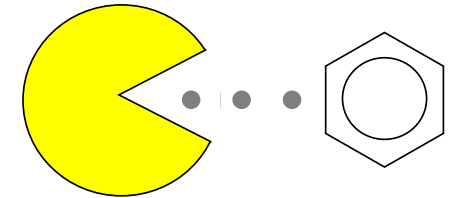
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aiming for?

toolbox development

database investigation

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- what additions are needed?



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overview

motivation

situation

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BIOREMEDIATION
using MULTIPLE
BACTERIAL SPECIES

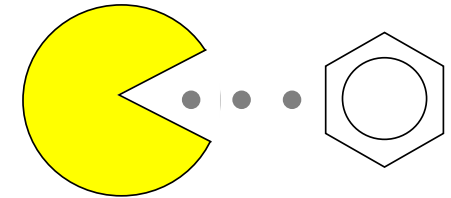
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aiming for?

toolbox development

database investigation

next steps

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- what are the **by-products** of pollutant mineralization?



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overview

motivation

situation

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BIOREMEDIATION
using MULTIPLE
BACTERIAL SPECIES

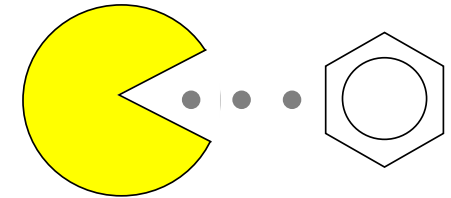
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aiming for?

toolbox development

database investigation

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- how can we take advantage of those bacteria?
- can't we use them for **facilitation of contaminat removal**?
- what additions are needed?
- what are the **by-products** of pollutant mineralization?
- what can we do about the by-products?



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overview

motivation

situation

idea: facilitation of
BIOREMEDIATION
using MULTIPLE
BACTERIAL SPECIES

idea: What are we
aiming for?

toolbox development

database investigation

next steps

■ input: **soil situation**

- pH
- humidity
- oxygen level
- temperature
- salinity
- present bacteria



idea: What are we aiming for?

overview

motivation

situation

idea: facilitation of
BIOREMEDIATION
using MULTIPLE
BACTERIAL SPECIES

idea: What are we
aiming for?

toolbox development

database investigation

next steps

■ input: **soil situation**

- pH
- humidity
- oxygen level
- temperature
- salinity
- present bacteria

■ desired **toolbox** output: **solution strategy**

- bacteria to introduce
- micronutrients to supply



overview

motivation

toolbox development

principle

technology

problems

database investigation

next steps

toolbox development



overview

motivation

toolbox development

principle

technology

problems

database investigation

next steps

- use knowledge from online databases

contaminatA



overview

motivation

toolbox development

principle

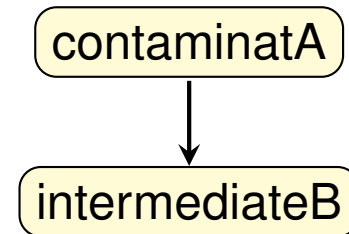
technology

problems

database investigation

next steps

- use knowledge from online databases
- search for **reactions** needed for degradation



overview

motivation

toolbox development

principle

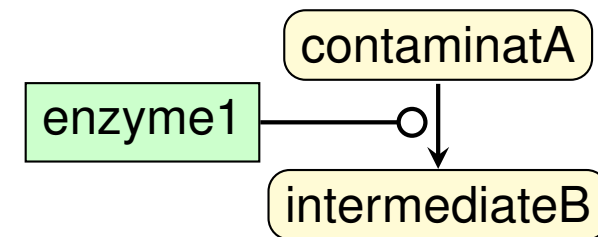
technology

problems

database investigation

next steps

- use knowledge from online databases
- search for **reactions** needed for degradation
- search **enzymes** for reactions



overview

motivation

toolbox development

principle

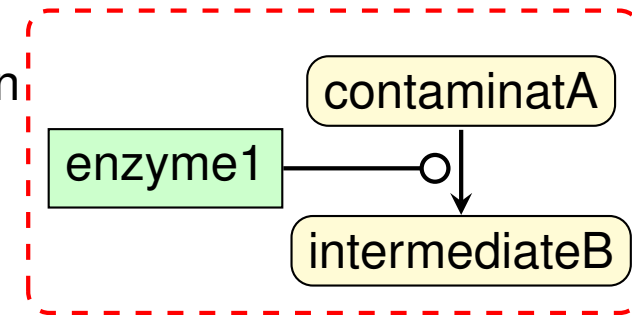
technology

problems

database investigation

next steps

- use knowledge from online databases
- search for **reactions** needed for degradation
- search **enzymes** for reactions
- search genes (\Rightarrow **bacteria**) for enzymes, assemble metabolic networks



overview

motivation

toolbox development

principle

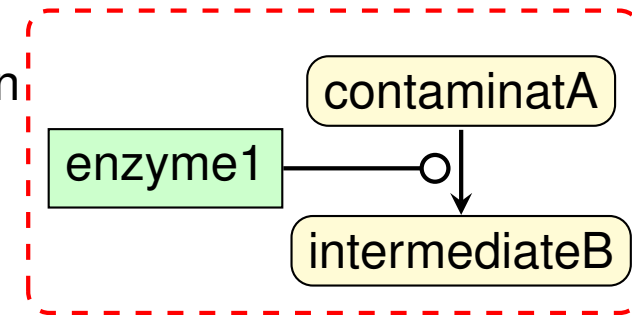
technology

problems

database investigation

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- use knowledge from online databases
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- calculate consumed and produced substances & intermediates



overview

motivation

toolbox development

principle

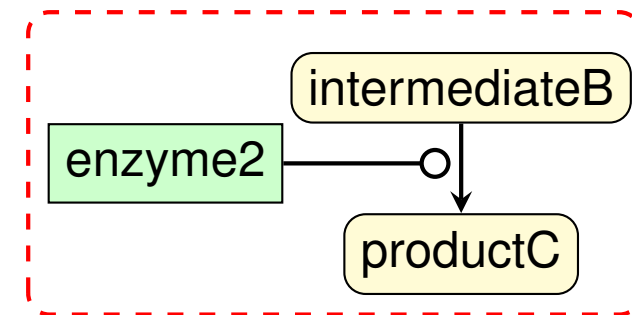
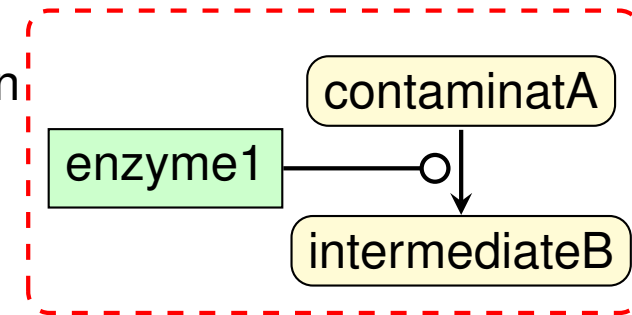
technology

problems

database investigation

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- repeat search for dead end products



overview

motivation

toolbox development

principle

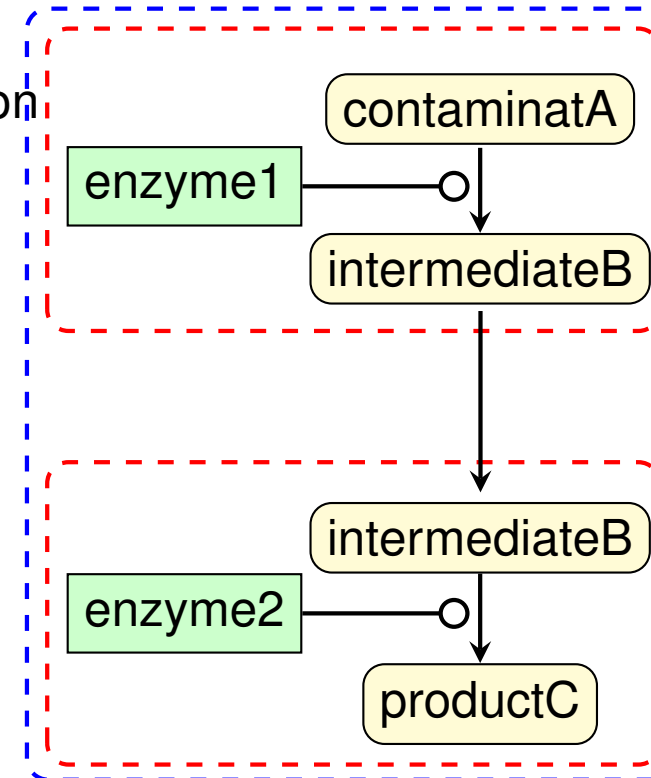
technology

problems

database investigation

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overview

motivation

toolbox development

principle

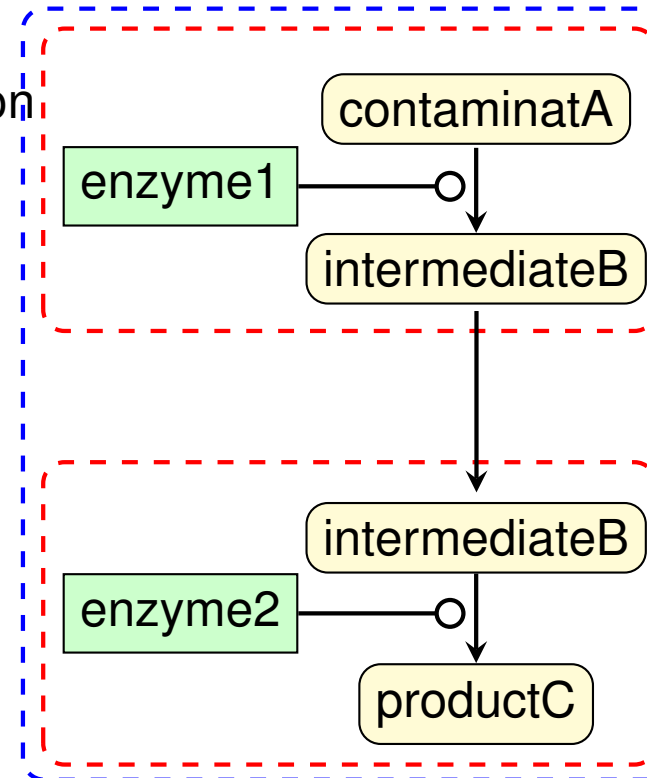
technology

problems

database investigation

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- use knowledge from online databases
- search for **reactions** needed for degradation
- search **enzymes** for reactions
- search genes (\Rightarrow **bacteria**) for enzymes, assemble metabolic networks
- calculate consumed and produced substances & intermediates
- repeat search for dead end products \Rightarrow **multi-species** bacterial networks
- may be done manually, but very complex



overview

motivation

toolbox development

principle

technology

problems

database investigation

next steps

- local **database integrates content** from online databases



overview

motivation

toolbox development

principle

technology

problems

database investigation

next steps

- local **database integrates content** from online databases
- calculation algorithms based on **graph theory** and **flux balance analysis**

overview

motivation

toolbox development

principle

technology

problems

database investigation

next steps

- local **database integrates content** from online databases
- calculation algorithms based on **graph theory** and **flux balance analysis**
- algorithms use numeric solvers (linear programming)!

overview

motivation

toolbox development

principle

technology

problems

database investigation

next steps

- local **database integrates content** from online databases
- calculation algorithms based on **graph theory** and **flux balance analysis**
- algorithms use numeric solvers (linear programming)!
- \Rightarrow calculation takes long times for whole-cell models

overview

motivation

toolbox development

principle

technology

problems

database investigation

next steps

- local **database integrates content** from online databases
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- \Rightarrow calculation takes long times for whole-cell models
- programs rely on **data accuracy**

overview

motivation

toolbox development

principle

technology

problems

database investigation

next steps

- local **database integrates content** from online databases
- calculation algorithms based on **graph theory** and **flux balance analysis**
- algorithms use numeric solvers (linear programming)!
- \Rightarrow calculation takes long times for whole-cell models
- programs rely on **data accuracy**
- \Rightarrow **prone to inconsistent data**

overview

motivation

toolbox development

principle

technology

problems

database investigation

next steps

■ missing annotations



overview

motivation

toolbox development

principle

technology

problems

database investigation

next steps

- missing annotations
- inconsistent **format** of data



overview

motivation

toolbox development

principle

technology

problems

database investigation

next steps

- missing annotations
- inconsistent **format** of data \Rightarrow high programming overhead



overview

motivation

toolbox development

principle

technology

problems

database investigation

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- missing annotations
- inconsistent **format** of data \Rightarrow high programming overhead
- inconsistent / **unbalanced reactions** in databases



overview

motivation

toolbox development

principle

technology

problems

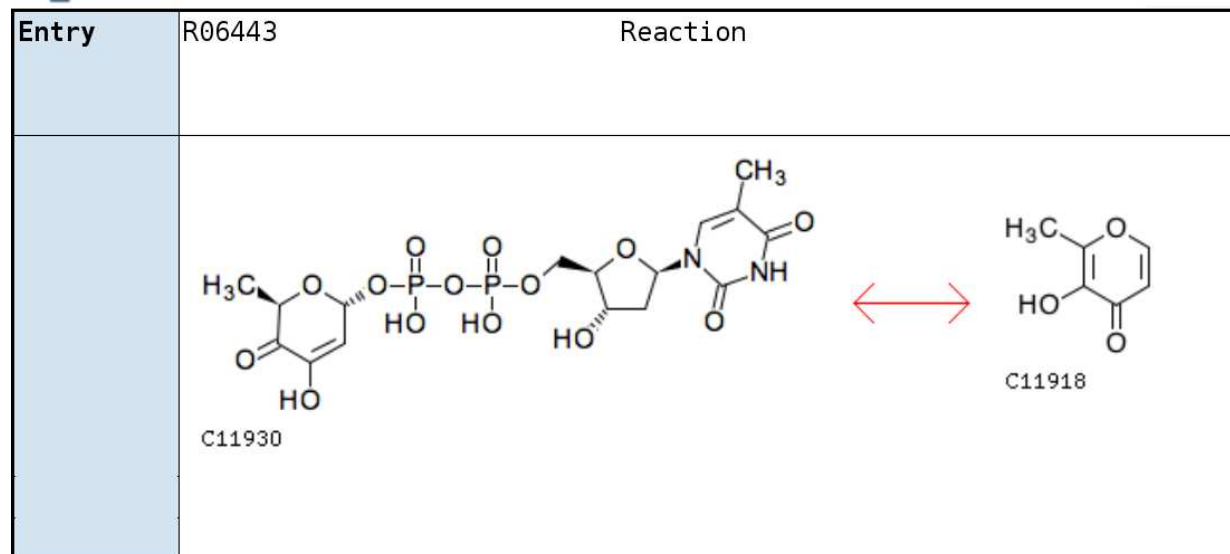
database investigation

next steps

- missing annotations
- inconsistent **format** of data \Rightarrow high programming overhead
- inconsistent / **unbalanced reactions** in databases

KfGG

REACTION: R06443



DBGET integrated database retrieval system

\Rightarrow inconsistent results



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overview

motivation

toolbox development

database investigation

inspection of
databases

database example:
KEGG
(Kyoto Encyclopedia of
Genes+Genomes)

KEGG Visit

next steps

database investigation

overview

motivation

toolbox development

database investigation

inspection of
databases

database example:
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KEGG Visit

next steps

- check links between entries / databases

overview

motivation

toolbox development

database investigation

inspection of
databases

database example:

KEGG

(Kyoto Encyclopedia of
Genes+Genomes)

KEGG Visit

next steps

- check links between entries / databases
- investigate completeness of annotation

overview

motivation

toolbox development

database investigation

inspection of
databases

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KEGG Visit

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overview

motivation

toolbox development

database investigation

inspection of
databases

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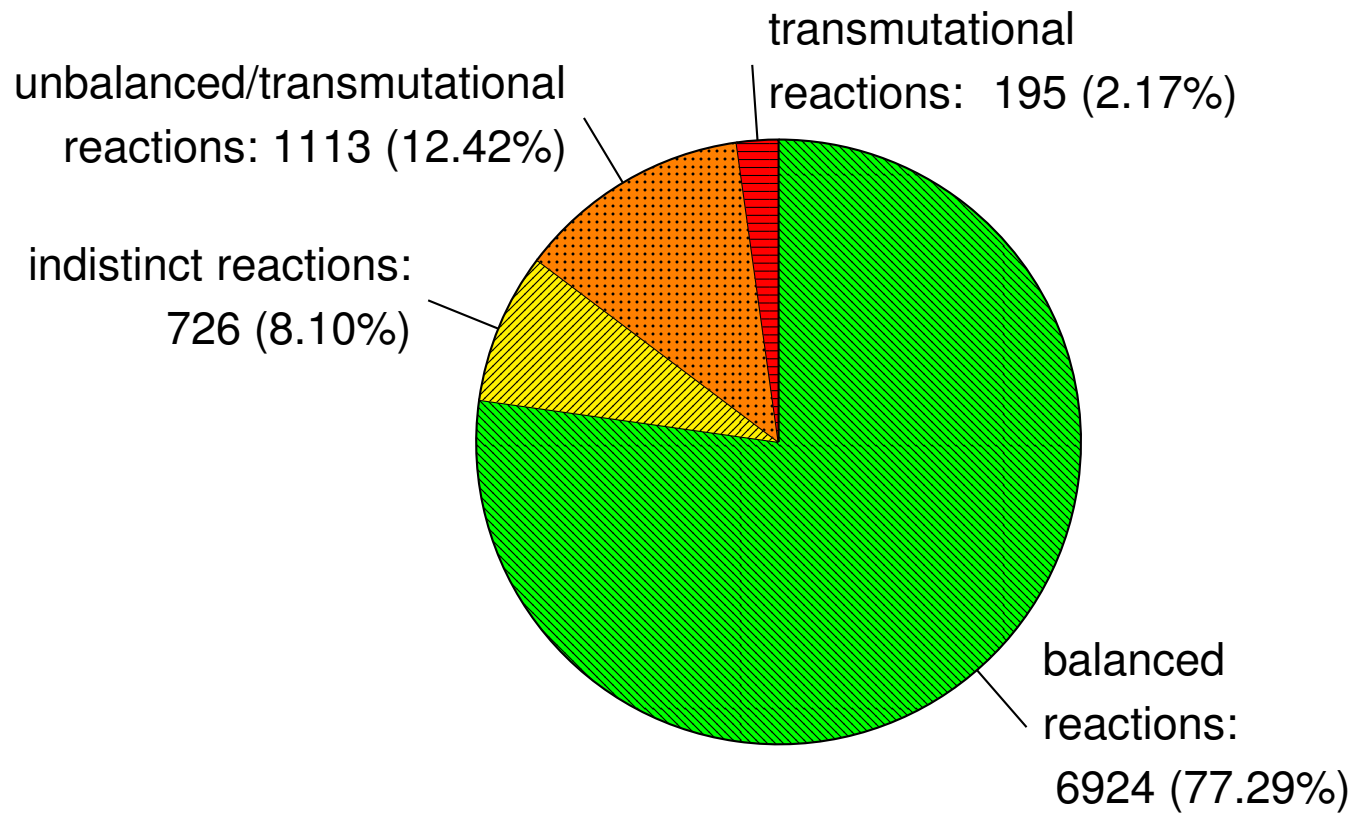
KEGG Visit

next steps

- check links between entries / databases
- investigate completeness of annotation
- check balance of reactions
- some inconsistencies may be automatically corrected

database example: KEGG (Kyoto Encyclopedia of Genes+Genomes)

- overview
- motivation
- toolbox development
- database investigation
- inspection of databases
- database example: KEGG (Kyoto Encyclopedia of Genes+Genomes)
- KEGG Visit
- next steps



overview on reaction inconsistencies in KEGG

overview

motivation

toolbox development

database investigation

inspection of
databases

database example:
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Genes+Genomes)

KEGG Visit

next steps

- visited Kyōto to learn more about the  database



overview

motivation

toolbox development

database investigation

inspection of
databases

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- exchange of ideas

overview

motivation

toolbox development

database investigation

inspection of
databases

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- exchange of ideas
- KEGG people incorporated corrections

overview

motivation

toolbox development

database investigation

next steps

publication

experiments

next steps

overview

motivation

toolbox development

database investigation

next steps

publication

experiments

- test our algorithm on curated data / networks
- publication of algorithm, results and ideas

overview

motivation

toolbox development

database investigation

next steps

publication

experiments

- test our algorithm on curated data / networks
- publication of algorithm, results and ideas
- release of software package for database analysis

overview

motivation

toolbox development

database investigation

next steps

publication

experiments

- cooperation with Institute for Theoretical Biology in Berlin

overview

motivation

toolbox development

database investigation

next steps

publication

experiments

- cooperation with Institute for Theoretical Biology in Berlin
- two-species experiments with particular Cyanobacteria stems and E.Coli

overview

motivation

toolbox development

database investigation

next steps

publication

experiments

thank you for your attention!



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