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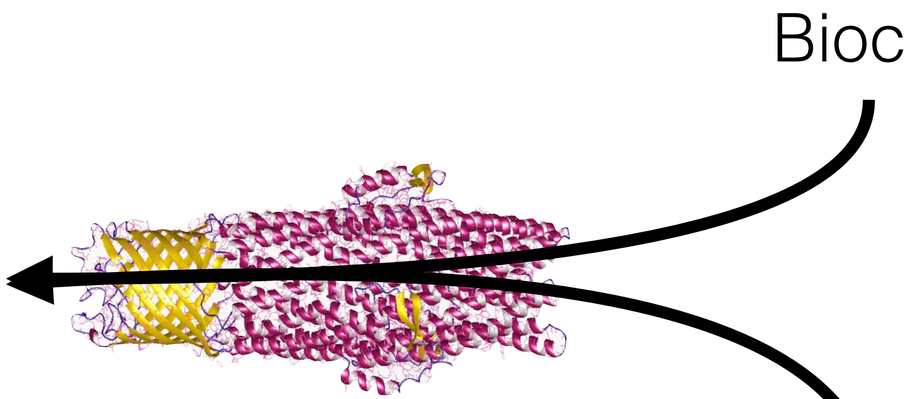
The BacMet database as a tool for biocide resistance risk assessment

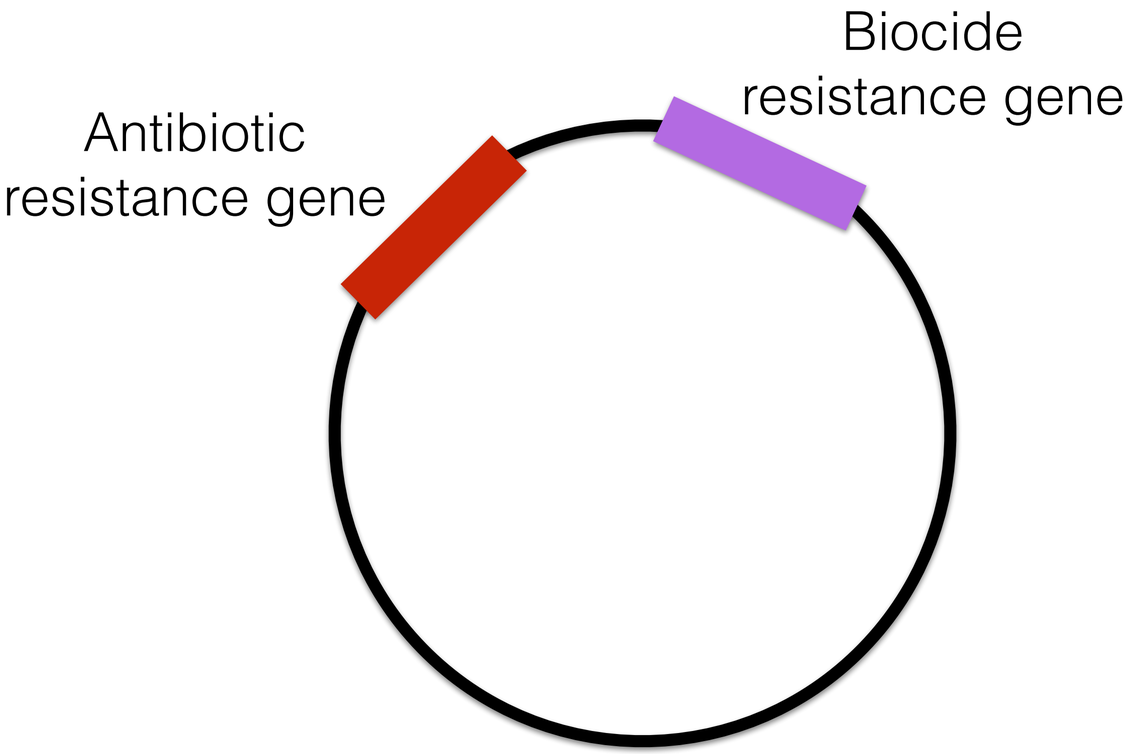
Johan Bengtsson-Palme

Biocide-antibiotic co-resistance



Biocide

Antibiotic



Deposition authors: Koronakis, V., Sharff, A.J., Koronakis, E., Luisi, B., Hughes, C.; visualization author: User:Astrojan - http://www.rcsb.org/pdb/explore/explore.do?structureId=1ek9

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BacMet: antibacterial biocide and metal resistance genes database

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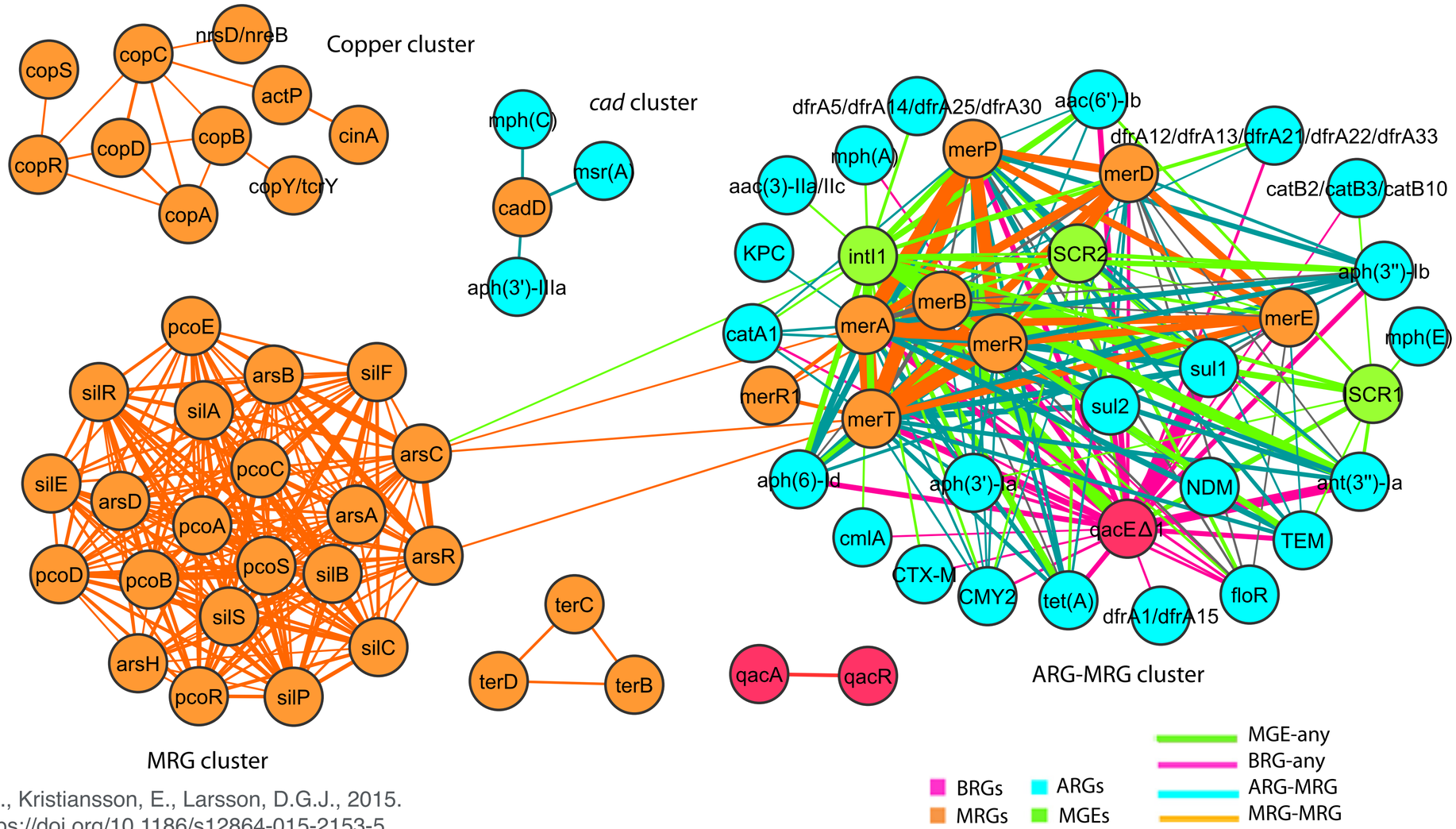
Gene co-occurences



Pal, C., Bengtsson-Palme, J., Kristiansson, E., Larsson, D.G.J., 2015.
BMC Genomics 16, 964. https://doi.org/10.1186/s12864-015-2153-5

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BacMet Demo

http://bacmet.biomedicine.gu.se/

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BacMet – Antibacterial Biocide & Metal Resistance Genes Database

BacMet is an easy-to-use bioinformatics resource of antibacterial biocide- and metal-resistance genes. BacMet consists of two databases:

- A manually curated database of genes with **experimentally confirmed** resistance function
- A database of **predicted** resistance genes based on sequence similarity to genes with experimentally confirmed function

Database Statistics (version 2.0)

Last updated: 11 March 2018

Predicted Resistance Genes: 155,512

Exp. Confirmed Resistance Genes: 753
- Chromosomal-borne: 550
- Plasmid/transposon-borne: 203

- Biocide resistance genes: 268
- Metal resistance genes: 420
- Genes with both biocide- and metal-resistance potential: 65

Total Compounds: 111
- Chemical classes: 43
- Antibacterial biocides: 58
- Metals: 23
- 'Other compounds' : 30

BacMet provides a high quality, manually curated database of bacterial genes that are experimentally confirmed to confer resistance to metals and/or antibacterial biocides, fully referenced to the scientific literature. BacMet also includes a database of predicted resistance genes, as the resistance genes may differ between species and/or occur in different forms that are not (yet) experimentally investigated. The database of predicted genes is generated by sequence similarity searches in public databases, using an uniform cut-off for genes found on plasmids, and individually set cut-offs for chromosomal genes.

BacMet provides tools for identification of biocide and metal-resistance genes in proteins and DNA sequences including full genomes. The genes in the databases can be accessed either through the browsing option, where one can browse genes by the compounds they confer resistance to or by their name. Alternatively one may use the search function to search for any term in the database, including for example gene name, name of biocide or metal and chemical class. Using the advanced search option, one may search specifically for e.g. plasmid-borne or chromosomal-borne genes. The entire database can also be downloaded for off-line analysis of larger datasets.

BacMet – Antibacterial Biocide & Metal Resistance Genes Database

HOME | BROWSE | SEARCH | BLAST | DOWNLOAD | ABOUT BacMet | SUBMISSION | TUTORIAL | FAQs | CONTACTS

- Experimentally Confirmed Database
  - By Biocides
  - By Metals
  - By other compounds
  - By Biocide Resistance Genes
  - By Metal Resistance Genes
  - By Genes that have both Biocide and Metal Resistance Potential
  - Total BacMet Experimentally Confirmed Database
- Predicted Database

B e of antibacterial biocide- and metal-resistance genes. BacMet consists of t

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- A database of **predic** sed on sequence similarity to genes with experimentally confirmed function

Database Statisti

Last updated: 1

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BacMet – Antibacterial Biocide & Metal Resistance Genes Database

Browsing Experimetal Confirmed database by biocides

Biocide Name	Chemical Class	Resistance Gene(s)
2-nitroimidazole	Imidazole	Click here
Acriflavine	Acridine	Click here
Alexidine	Biguanides	Click here
Benzylkonium Chloride (BAC)	Quaternary Ammonium Compounds (QACs)	Click here
Cetrimide (CTM)	Quaternary Ammonium Compounds (QACs)	Click here
Cetylpyridinium Chloride (CPC)	Quaternary Ammonium Compounds (QACs)	Click here
Chlorhexidine	Biguanides	Click here
Clorine Dioxide (ClO2)	Halogens	Click here
Crystal Violet	Triarylmethane	Click here
Dequalinium chloride	Quaternary Ammonium Compounds (QACs)	Click here
Dibrompropamidine	Diamidine	Click here
Dodine	Acetate	Click here
Diphenyl Ether	Phenyl	Click here
Empigen	Amine betaine	Click here
Ethidium Bromide	Phenanthridine	Click here
Ethylbenzene	Aromatic hydrocarbons	Click here
Ethylmercury chloride	Organo-mercury	Click here
Glycerol	Alcohol	Click here
Hexamidine	Diamidine	Click here
Hydrochloric Acid (HCl)	Acid	Click here
Hydrogen Peroxide (H2O2)	Peroxides	Click here
Linoleic acid	Free Fatty Acids	Click here
m-xylene	Aromatic hydrocarbons	Click here
Methylene Blue	Thiazinium	Click here

Browsing BacMet compounds

Information of 2-nitroimidazole from BacMet

Compound Information

- **Compound name:** 2-nitroimidazole
- **Chemical Class:** Imidazole
- **Description:** It is an industrial biocide. It is only effective against anaerobic organisms and it is effective against sulfate-reducing bacteria (SRB) and compatible with other chemicals. Used to prepare nitroimidazole substituted boronic acids as precursors for imaging hypoxic tissue. Also used to prepare potential site-selective radiosensitizers for estrogen receptor-rich tumors.
- **Database Links:** CHEBI:67135

BacMet – Antibacterial Biocide & Metal Resistance Genes Database

Browsing Experimentally Confirmed database

Result: Your query found 1 resistance gene(s) from the BacMet Experimentally Confirmed database

Gene_name	Experimentally Verified Resistance Gene Information	Predicted Resistance Gene Information
ruvB	• **BacMet ID:** BAC0293 • **Code for:** Enzyme • **Family:** Malic enzymes family • **Sequence:** FASTA • **Cross-database IDs:** Link • **Organism:** *Pseudomonas corrugata 28* • **Location:** Chromosome • **Compound:** Chromium (Cr), Cetylpyridinium Chloride (CPC) [class: Quaternary Ammonium Compounds (QACs)], Dodine [class: Acetate], 2-nitroimidazole [class: imidazole] • **Description:** It is a fragment of ruvB gene product. It is a oxidoreductase from malic enzyme family. • **Length (amino acid):** 379 • **Reference:** Decorosi et al. 2009; Pubmed- 19768364	Similar resistance genes in 'BacMet Predicted database'

BacMet database and website is designed and maintained by Chandan Pal

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BacMet Predicted Database

Result: Your query found 495 resistance gene(s) from the BacMet Predicted database

Gene name	GI number	GenBank ID	Sequence	Organism	Compound	NCBI annotation
ruvB	15596164	NP_249658.1	FASTA	*Pseudomonas aeruginosa PAO1*	Chromium (Cr), Tellurium (Te), Selenium (Se)	ruvB gene product
ruvB	7443650	PIR: JC5477	FASTA	*Pseudomonas aeruginosa*	Chromium (Cr), Tellurium (Te), Selenium (Se)	DNA-binding protein ruvB - Pseudomonas aeruginosa
ruvB	1183842	BAA11819.1	FASTA	*Pseudomonas aeruginosa*	Chromium (Cr), Tellurium (Te), Selenium (Se)	Holliday junction specific DNA helicase
ruvB	152988470	YP_001349890.1	FASTA	*Pseudomonas aeruginosa PA7*	Chromium (Cr), Tellurium (Te), Selenium (Se)	Holliday junction DNA helicase RuvB
ruvB	289674672	ZP_06495562.1	FASTA	*Pseudomonas syringae pv. syringae FF5*	Chromium (Cr), Tellurium (Te), Selenium (Se)	Holliday junction DNA helicase RuvB
ruvB	28871122	NP_793741.1	FASTA	*Pseudomonas syringae pv. tomato str. DC3000*	Chromium (Cr), Tellurium (Te), Selenium (Se)	Holliday junction DNA helicase RuvB
ruvB	289626497	ZP_06459451.1	FASTA	*Pseudomonas syringae pv. aesculi str. NCPPB 3681*	Chromium (Cr), Tellurium (Te), Selenium (Se)	Holliday junction DNA helicase RuvB
ruvB	237800219	ZP_04588680.1	FASTA	*Pseudomonas syringae pv. oryzae str. 1_6*	Chromium (Cr), Tellurium (Te), Selenium (Se)	Holliday junction DNA helicase RuvB
ruvB	71736556	YP_275912.1	FASTA	*Pseudomonas syringae pv. phaseolicola 1448A*	Chromium (Cr), Tellurium (Te), Selenium (Se)	Holliday junction DNA helicase RuvB
				Pseudomonas	Chromium (Cr), Tellurium	

Query BacMet databases

1. Quick Search:

You can search the BacMet database using any full term or partial term with a wildcard, including for example gene names (e.g. copA or cop*), name of biocides (e.g. Triclosan or Triclo*), metals (e.g. Arsenic or Arsen*) or chemical classes (e.g. Acridine or Acrid*). You will get an output in a table format with the resistance gene information that matches to your search term/pattern.

EXP Confirmed Database Search

Predicted Database Search

2. Advanced Search:

You can use the advanced search option if you are especially interested in resistance genes that confer resistance to certain antibacterial compounds or chemical classes, and plasmid- or chromosomal-borne resistance genes. You can use full term or partial term with a wildcard in description section (e.g. resistance or resis*).You will get an output in a table format with the resistance gene information that matches to your search criteria.

Select 'chemical class'/'compound' (resistant to): class: Any

Select location: Any Chromosome Plasmid (for EXP confirmed database only)

Protein description contains text (e.g. resistance)

Peptide sequence length greater than 50 (for EXP confirmed database only)

Peptide sequence length less than 2000 (for EXP confirmed database only)

Select database: BacMet Predicted database BacMet Experimentally Confirmed database

Moving towards a risk assessment tool

- Incorporate data on **selective concentrations** and **co-selection opportunities**
- Make BacMet useful for practical risk assessment and management

BacMet Update

- Current data will remain and be expanded upon
- **Substance-based** rather than gene-based focus – commonly the starting point for risk assessment
- **MICs and LOECs** for different species, PNECs for resistance selection and HGT
- **New genes** will be added (from literature and this project)
- **Context information** (hosts, mobility potential, co-location with other resistance genes), based on available genome data
- Relative **abundance in different environment types**

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Acknowledgement

- Chandan Pal
- Joakim Larsson
- Erik Kristiansson
- Christopher Rensing
- Funding from FORMAS

Discussion tasks

Short introduction round (3-4 sentences per person)

http://bacmet.biomedicine.gu.se/

Who takes the minutes?

How can the BacMet database support biocide resistance risk assessment during approval/ authorization of biocides?

What needs to be changed to be able to use the BacMet database for the regulatory process?

Proposed structural changes?

Proposed new categories?

Proposed links with other relevant databases?

BacMet currently is a substance-based database. How to incorporate results for products?

Who would like to present the results?