ANTIBIOTICS DATABANK

Final Project Report

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Abstract

Over ten weeks I have worked to implement an antibiotics databank, with methods of viewing, collating and entering data. At the end of the project, the infrastructure is complete, with a database schema that, while probably not even close to final, is serviceable for the current iteration. In addition, PHP-generated html gives a web-based interface to retrieve data, and there is an interface for direct data-entry under development. Contained within is a detailed breakdown of each section, and appendices containing technical information and visual proof of the progress made.

Introduction

With the rise of antibiotic resistance, there is ever increasing demand for tools to assist antibiotics research. We are building the Antibiotics Databank, the first ever systematic collection of antibiotics research evidence. As a first step we will create a database of research evidence about combination antibiotics. This project will develop the necessary database and supporting tools to enable researchers to enter evidence into the database and perform useful queries of it.

This is the introduction given to the project when I first embarked upon it, and it seems only reasonable to include it here as an introduction. Over ten weeks, I have aimed to fulfill the requirements laid upon me by this one paragraph, and while I do not feel like the time given was long enough (and I believe it was understood that I would not be expected to have a finished piece in the time available), I am very satisfied with what I have achieved.

This report serves as a documentation of the progress I have made, and a summary of the state of the project after ten weeks.

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Database Schema

The initial step in designing the system was to decide on the infrastructure hosting the database itself. After consultation with others, and with the almighty Google, the easiest system to integrate into a web-host seemed to be a MySQL Server. This also highlights the need for a web-host; fortunately, a friend of mine has a private server that he was able to lend me control of for the duration of the project.

Once the server was set up, running Linux, Apache Web Services, MySQL Server and PHP (a LAMP configuration), the next task was to determine the organizational structure for the data. Once the links between datasets has been determined, it can be used to inform the structure of the interface to follow the same logical lines. By this point in the project, there are 24 tables within the database, which can be placed under five categories: antibiotics; classes; combinations; studies; and the rest (aka miscellanea, for tables with subsidiary information). There is one table to link between combinations and antibiotics which falls under both, but all other tables are distinct. Below is a list of tables, with a brief overview of their function and/or contents separated by category.

See Appendix 1 for the full schema.

Antibiotics

The data for each antibiotic was taken from http://en.wikipedia.org/wiki/List_of_antibiotics, with additional information harvested from individual Wikipedia articles for each antibiotic.

antibiotics

Contains the information for a single antibiotic, along with a link to the class.

antibiotic_atc_codes

A many-to-one relationship of Anatomical Therapeutic Chemical (ATC) codes to antibiotics, as defined by the World Health Organisation Collaborating Centre for Drug Statistics Methodology (WHOCC).

antibiotic_brand_names

A many-to-one relationship of brand names to antibiotics.

combination_antibiotic_link

A many-to-many link table of antibiotics to combinations in which they are constituent, along with the proportions of each antibiotic in each combination. This table links to the combination table.

common_use_antibiotic_link

A many-to-many link of common uses to antibiotics. This table links to the common_uses table.

mechanism_antibiotic_link

A many-to-one link of mechanisms to antibiotics. This table links to the mechanisms table.

side_effect_antibiotic_link

A many-to-many link of side effects to antibiotics, and the likelihood of them occurring. This table links to the side_effects and likelihood tables.

Classes

The data for each class was taken from the same Wikipedia article as antibiotics, with judgment being used to determine which values for common uses, mechanisms, and side effects should be entered as default for the class.

classes

Contains the names of the various classes of antibiotics.

common_use_class_link

A many-to-many link of common uses to classes, for use in pre-populating new antibiotic records. This table links to the common_uses table.

mechanism_class_link

A many-to-many link of mechanisms to classes, for use in pre-populating new antibiotic records. This table links to the mechanisms table.

side_effect_class_link

A many-to-many link of side effects to classes, for use in pre-populating new antibiotic records, and the likelihood of them occurring. This table links to the side_effects and likelihood tables.

Combinations

The data for this section is considerably more sparse, and is expected to be the major area for further data input. The data at this time consists of the few combinations included in Wikipedia's list of antibiotics.

combinations

Contains the names of the various combinations of antibiotics.

combination_antibiotic_link

See combination_antibiotic_link under Antibiotics.

combination_brand_names

A many-to-one relationship of brand names to combinations.

combination_treatment_link

A many-to-many relationship of combinations to treatments. This table links to the treatments table.

Studies

At time of writing, one study had been (partially) entered into the database. The study (provided by Jiangning Song) is used primarily here as a placeholder to allow viewing of the screens. The schema for this section should not be considered final. See Further Work for more information.

study

Contains the name of the study, a link to the ID of the combination or antibiotic on which the study was performed, a marker to indicate whether it was a combination or pure antibiotic subject, and a link to the PubMed ID of the study itself.

isolates

A many-to-one relationship of the sources of culture on which the study was performed. Contains a link to the species being studied for each source.

Miscellanea

This section groups the remaining tables that contain subsidiary information.

common_uses

Contains a list of maladies and ailments that one might wish to treat with antibiotics, to be linked to antibiotics and classes thereof.

likelihood

Contains a list of both general and specific rates of occurrence (e.g. common, uncommon, when mixed with alcohol, etc.), to be linked with side effects and then to antibiotics and classes.

mechanisms

Contains a list of processes that any given antibiotic or class of antibiotic may either inhibit or promote, in order to give treatment. These are to be linked to antibiotics and classes.

side_effects

Contains a list of possible side effects (e.g. nausea, headaches, etc.) to be paired with a likelihood and linked to antibiotics and classes.

species

Contains a list of bacterial species for use by the isolates table.

time_kill_series

A many-to-one relationship of time-kill kinetic data to each isolate, including the concentration used.

treatments

Contains a list of treatments, for use by the combinations table.

urls

A system table, used to maintain the hyperlinks to external sites. Should a website change its url format, this table can be used to update the databank without having to change hardcoded values.

Databank Viewing

Once the structure of the database had been determined to a reasonable degree (fully in the knowledge that it would require extension and revision), it was time to begin the task of designing and implementing the end-user interaction. My initial idea was to replicate the look and feel of a manila folder, with information represented in tabs and sub-tabs. As such, I sketched the mock-ups seen in Appendix 2, and took them to Dr. Song for approval. After some discussion, and some minor modifications, the process of converting them into working web pages could begin.

The pages themselves are presented to the user as pure html, but are generated by PHP scripts running on the server, which generate the html from assembling pre-prepared and dynamically created sections. Each category of page (antibiotics, classes, combinations, and studies) has a set of common functions to create interior tab rows, which fall back to a generalised common set of routines to do the page header and footer, the top tab row, general headers and sub-headers, etc.

Data is retrieved through tailored SQL statements, and (for the directories) iterated through in three columns or (for the info pages) iterated through to find the record to allow for finding the previous and next records as well to generate the navigation links.

Every page is almost entirely composed of a single table, with 9 columns. Turning borders on and off depending on the location of each cell allows us to hide the true nature of the table, while still allowing for consistent positioning of elements by placing them in specific columns (or sets of columns, by merging adjacent cells).

Each directory page is a single 'pane', subdivided (if necessary) by headers. Each info page has a navigation section, a header and a sub-header, followed by a tab bar for this category. Each tab is technically a separate page, although the top pane remains the same. The lower pane changes depending on the selected tab.

All pages in the viewing section are styled by the same CSS (cascading style-sheets), to give a consistent look across the databank. The primary colour is yellow (specifically #FFFFBB, so a fairly pale yellow), with even paler yellow being used for unselected tabs. The classes in the style sheet allow for fine adjustment of alignment and look of any given element in the table (including, but not limited to: text alignment, bold, italics, size and font, left and right borders and background colour).

Screenshots of all screens at the present time can be seen in Appendix 3.

Databank Editing

There is currently only one way to edit the database, with a more user-friendly way in mid-development at time of writing.

Direct database access is available through the phpMyAdmin database administration. This interface allows the greatest control over the database contents, but is not greatly intuitive, due to its dependence on remembering IDs between editing different tables.

The method currently in development utilises the links between data to allow in situ selection of values through drop downs. PHP post requests will then be used to parse and edit / insert / delete the appropriate records. Currently, the interface is mostly complete, with the backend logic laid out but not implemented.

Both methods of editing the database can be seen in Appendix 4.

Conclusions

Progress

In 10 weeks, this project has gone from an idea to a mostly-realised usable system. A database has been implemented, a full web structure is now in place, and the editing system is coming together nicely. Progress was initially rapid, but in the last few weeks, a glut of assignments caused a regrettable slow down, leading to a fair amount of elements that would have been nice to have, being unfinished. That being said, the structure lends itself to extensibility. With a full comment sweep, it should be entirely feasible for the project to be picked up by someone with a decent understanding of databases, PHP and html.

Learning Outcomes

At the beginning of this project, I had a suitable understanding of html syntax, CSS, and Unix systems. At this point, I now have a much better understanding of html and CSS, along with more experience. I am now confident in writing PHP, I understand Apache web services a little more, and I have had a little more practice in administration of databases (although this has been a skill of mine through my employment for the last four years). I also have had more practice in formal report writing.

Reflections

This project has been very enjoyable, and useful in terms of skill development. I have developed a system I am proud to call my own, and intend to add it to my portfolio of projects for future employers.

Further Work

While a lot of progress has been made with the databank thus far, there remains a lot of work to be done.

Data

While the antibiotics and class information are well populated, the combinations and studies pages are virtually blank. A concerted effort will be required to input data to a point where the databank is usable.

The database will need to continue being revised, as new requirements are identified. In particular, the tables relating to the study section are almost certainly over simplistic, and will need to be extended as more data classifications are differentiated.

The common uses and mechanisms tables are currently blank, awaiting the simplification of data from Wikipedia into keywords that can be allocated independently, rather than dense paragraphs of text unique to any given antibiotic. This will require input from someone with expertise in the field.

Basic Functionality

The studies pages are woefully incomplete, due to insufficient time and prioritisation of basic editing infrastructure. The decision was made to lay the groundwork for the editing page (which uses a very different logic set and layout to any other page) rather than implement the studies page which, at its heart, is very similar to the pages already in place for antibiotics, classes, and combinations.

The editing section itself is also incomplete, and will require a significant amount of effort to complete. Basic functionality can be achieved by following the structure in place and implementing the backend, but it would be much more user-friendly if some JavaScript or similar could be implemented to increase the flexibility of the input system.

There are also sections that are incomplete due to insufficient experience on my part with the field to identify critical information. User feedback will be critical in identifying missing fields and information.

Finally, it would be useful to implement a panel for statistics, to report on the data bank as a whole, but this is very much a bonus, as opposed to necessary functionality.

Aesthetics

In terms of display, there remains something to be desired in terms of aesthetic appeal. Currently fields are laid out in a functional way, but, due to unfamiliarity with the base material, they have not been organised to place more important information in a more visible location. Again, once a would-be user has had a chance to investigate the system, there should be sufficient feedback to commence reorganisation.

The CSS currently is rather basic, and could probably benefit from some sparkly bits to improve the overall look of the site, and possibly bring it more in line with Monash style guides.

Infrastructure

The current hosting system is untenable – a permanent home needs to be found for the databank on a suitable server. This will require a full backup of the database and all PHP files, followed by a curated migration to its new host.

Appendices

Appendix 1: Full Database Schema

antibiotics

Column	Type
ID	int(11)
NAME	varchar(60)
CLASS_ID	int(11)
CHEMSPIDER_ID	varchar(60)
CAS_NUMBER	varchar(60)
PUBCHEM_ID	varchar(60)
IUPHAR	varchar(60)
DRUGBANK_ID	varchar(60)
UNII	varchar(60)
KEGG	varchar(60)
CHEBI	varchar(60)
CHEMBL	varchar(60)
FORMULA	varchar(60)
MOLECULAR_MASS	float

Keyname	Column	Unique
ID	ID	Yes
NAME	NAME ID	Yes
CLASS_ID	CLASS_ID ID	Yes

antibiotic_atc_codes

Column	Type
ID	int(11)
ANTIBIOTIC_ID	int(11)
CODE	varchar(60)

Keyname	Column	Unique
ID	ID	Yes
ANTIBIOTIC_ID	ANTIBIOTIC_ID ID	Yes

antibiotic_brand_names

Column	Type
ID	int(11)
ANTIBIOTIC_ID	int(11)
NAME	varchar(60)
DISCONTINUED	tinyint(1)

Keyname	Column	Unique

Keyname	Column	Unique
ID	ID	Yes
ANTIBIOTIC_ID	ANTIBIOTIC_ID	Yes
	ID	

classes

Column	Type
ID	int(11)
NAME	varchar(60)

Keyname	Column	Unique
ID	ID	Yes
NAME	NAME	No

combinations

Column	Type
ID	int(11)
NAME	varchar(150)

Keyname	Column	Unique
ID	ID	Yes
NAME	NAME	Yes
	ID	

combination_antibiotic_link

Column	Type
ID	int(11)
COMBINATION_ID	int(11)
ANTIBIOTIC_ID	int(11)
PROPORTION	float

Keyname	Column	Unique
ID	ID	Yes
COMBINATION_ID + ANTIBIOTIC_ID	COMBINATION_ID	Yes
	ANTIBIOTIC_ID	
	ID	
ANTIBIOTIC_ID + COMBINATION_ID	ANTIBIOTIC_ID	Yes
	COMBINATION_ID	
	ID	

combination_brand_names

Column	Type
ID	int(11)
COMBINATION_ID	int(11)
NAME	varchar(60)

Keyname	Column	Unique

	ID	Yes
ID	ID	Yes
COMBINATION_ID	COMBINATION_ID	Yes
	ID	

combination_treatment_link

Column	Type
ID	int(11)
COMBINATION_ID	int(11)
TREATMENT_ID	int(11)

Keyname	Column	Unique
ID	ID	Yes
COMBINATION_ID +	COMBINATION_ID	Yes
TREATMENT_ID	TREATMENT_ID	
	ID	
TREATMENT_ID +	TREATMENT_ID	Yes
COMBINATION_ID	COMBINATION_ID	
	ID	

common_uses

Column	Type
ID	int(11)
TEXT	varchar(100)

Keyname	Column	Unique
ID	ID	Yes

common_use_antibiotic_link

Column	Type
ID	int(11)
ANTIBIOTIC_ID	int(11)
COMMON_USE_ID	int(11)

Keyname	Column	Unique
ID	ID	Yes
ANTIBIOTIC_ID +	ANTIBIOTIC_ID	Yes
COMMON_USE_ID	COMMON_USE_ID	
	ID	
COMMON_USE_ID +	COMMON_USE_ID	Yes
ANTIBIOTIC_ID	ANTIBIOTIC_ID	
	ID	

common_use_class_link

Column	Type
ID	int(11)
CLASS_ID	int(11)

COMMON_USE_ID   int(11)

Keyname	Column	Unique
ID	ID	Yes
CLASS_ID + **COMMON_USE_ID**	CLASS_ID COMMON_USE_ID ID	Yes
COMMON_USE_ID + **CLASS_ID**	COMMON_USE_ID CLASS_ID ID	Yes

isolates

Column	Type
ID	int(11)
STUDY_ID	int(11)
SPECIES_ID	int(11)
SOURCE	varchar(100)

Keyname	Column	Unique
ID	ID	Yes
STUDY_ID + SPECIES_ID	STUDY_ID SPECIES_ID ID	Yes
SPECIES_ID + STUDY_ID	SPECIES_ID STUDY_ID ID	Yes

likelihood

Column	Type
ID	int(11)
NAME	varchar(30)

Keyname	Column	Unique
ID	ID	Yes

mechanisms

Column	Type
ID	int(11)
TEXT	varchar(100)

Keyname	Column	Unique
ID	ID	Yes

mechanism_antibiotic_link

Column	Type
ID	int(11)

ANTIBIOTIC_ID	int(11)
MECHANISM_ID	int(11)

Keyname	Column	Unique
ID	ID	Yes
ANTIBIOTIC_ID + MECHANISM_ID	ANTIBIOTIC_ID MECHANISM_ID ID	Yes
MECHANISM_ID + ANTIBIOTIC_ID	MECHANISM_ID ANTIBIOTIC_ID ID	Yes

mechanism_class_link

Column	Type
ID	int(11)
CLASS_ID	int(11)
MECHANISM_ID	int(11)

Keyname	Column	Unique
ID	ID	Yes
CLASS_ID + MECHANISM_ID	CLASS_ID MECHANISM_ID ID	Yes
MECHANISM_ID + CLASS_ID	MECHANISM_ID CLASS_ID ID	Yes

side_effects

Column	Type
ID	int(11)
TEXT	text

Keyname	Column	Unique
ID	ID	Yes

side_effect_antibiotic_link

Column	Type
ID	int(11)
ANTIBIOTIC_ID	int(11)
SIDE_EFFECT_ID	int(11)
LIKELIHOOD_ID	int(11)

Keyname	Column	Unique
ID	ID	Yes
	ANTIBIOTIC_ID	Yes

Keyname	Column	Unique
ANTIBIOTIC_ID + SIDE_EFFECT_ID	SIDE_EFFECT_ID ID	
SIDE_EFFECT_ID + ANTIBIOTIC_ID	SIDE_EFFECT_ID ANTIBIOTIC_ID ID	Yes

side_effect_class_link

Column	Type
ID	int(11)
CLASS_ID	int(11)
SIDE_EFFECT_ID	int(11)
LIKELIHOOD_ID	int(11)

Keyname	Column	Unique
ID	ID	Yes
CLASS_ID + SIDE_EFFECT_ID	CLASS_ID SIDE_EFFECT_ID ID	Yes
SIDE_EFFECT_ID + CLASS_ID	SIDE_EFFECT_ID CLASS_ID ID	Yes

species

Column	Type
ID	int(11)
NAME	varchar(60)

Keyname	Column	Unique
ID	ID	Yes

study

Column	Type
ID	int(11)
ENTITY_ID	int(11)
ENTITY_TYPE	varchar(1)
PUBMED_ID	int(11)
NAME	varchar(100)

Keyname	Column	Unique
ID	ID	Yes
NAME	NAME ID	Yes
ENTITY_ID + NAME	ENTITY_ID NAME ID	Yes

time_kill_series

Column	Type
ID	int(11)
ISOLATE_ID	int(11)
FIC	double
TIME_MIN	int(11)
CONCENTRATION	double

Keyname	Column	Unique
ID	ID	Yes
	ISOLATE_ID	
ISOLATE_ID + FIC +	FIC	
CONCENTRATION +	CONCENTRATION	Yes
TIME_MIN	TIME_MIN	
	ID	

treatments

Column	Type
ID	int(11)
NAME	varchar(60)

Keyname	Column	Unique
ID	ID	Yes

urls

Column	Type
CHEMSPIDER_IMAGE_START	varchar(100)
CHEMSPIDER_IMAGE_END	varchar(100)
CAS_NUMBER_START	varchar(100)
CAS_NUMBER_END	varchar(100)
PUBCHEM_ID_START	varchar(100)
PUBCHEM_ID_END	varchar(100)
DRUGBANK_ID_START	varchar(100)
DRUGBANK_ID_END	varchar(100)
KEGG_START	varchar(100)
KEGG_END	varchar(100)
UNII_START	varchar(100)
UNII_END	varchar(100)
CHEBI_START	varchar(100)
CHEBI_END	varchar(100)
CHEMBL_START	varchar(100)
CHEMBL_END	varchar(100)
IUPHAR_START	varchar(100)
IUPHAR_END	varchar(100)
ATC_START	varchar(100)
ATC_END	varchar(100)

WIKIPEDIA_START	varchar(100)
WIKIPEDIA_END	varchar(100)
CHEMSPIDER_ID_START	varchar(100)
CHEMSPIDER_ID_END	varchar(100)
PUBMED_ID_START	varchar(100)
PUBMED_ID_END	varchar(100)

Appendix 2: Initial Sketches
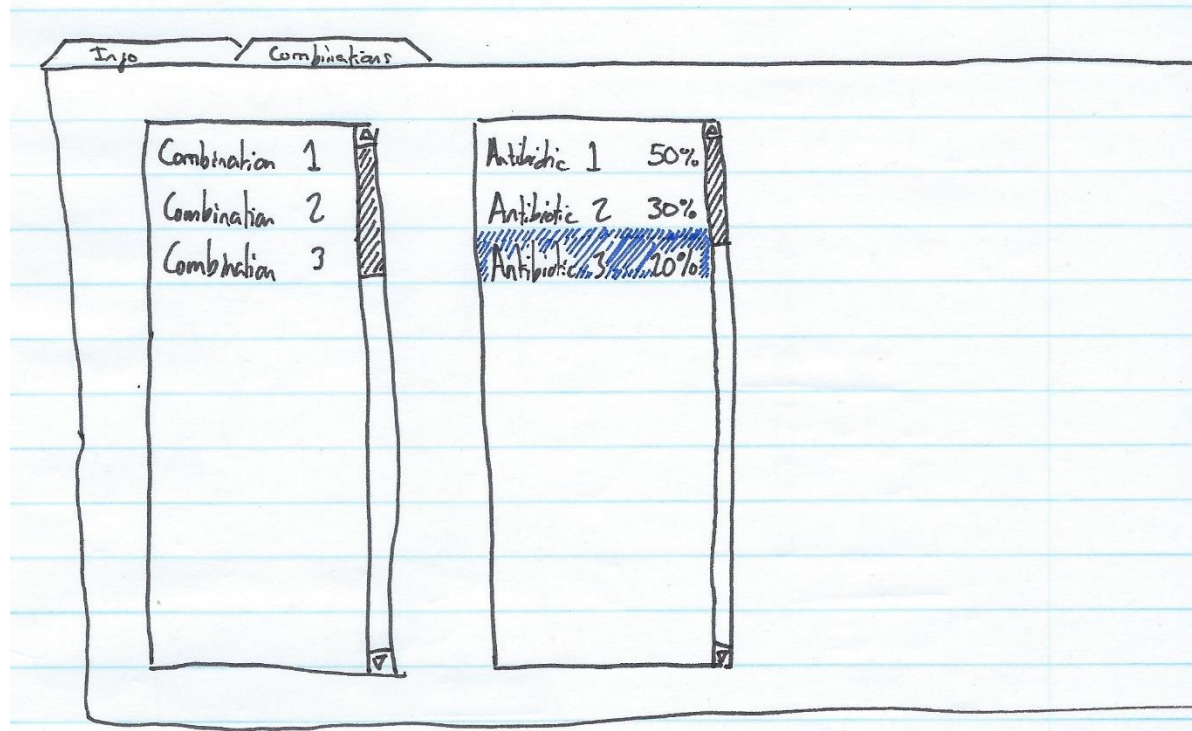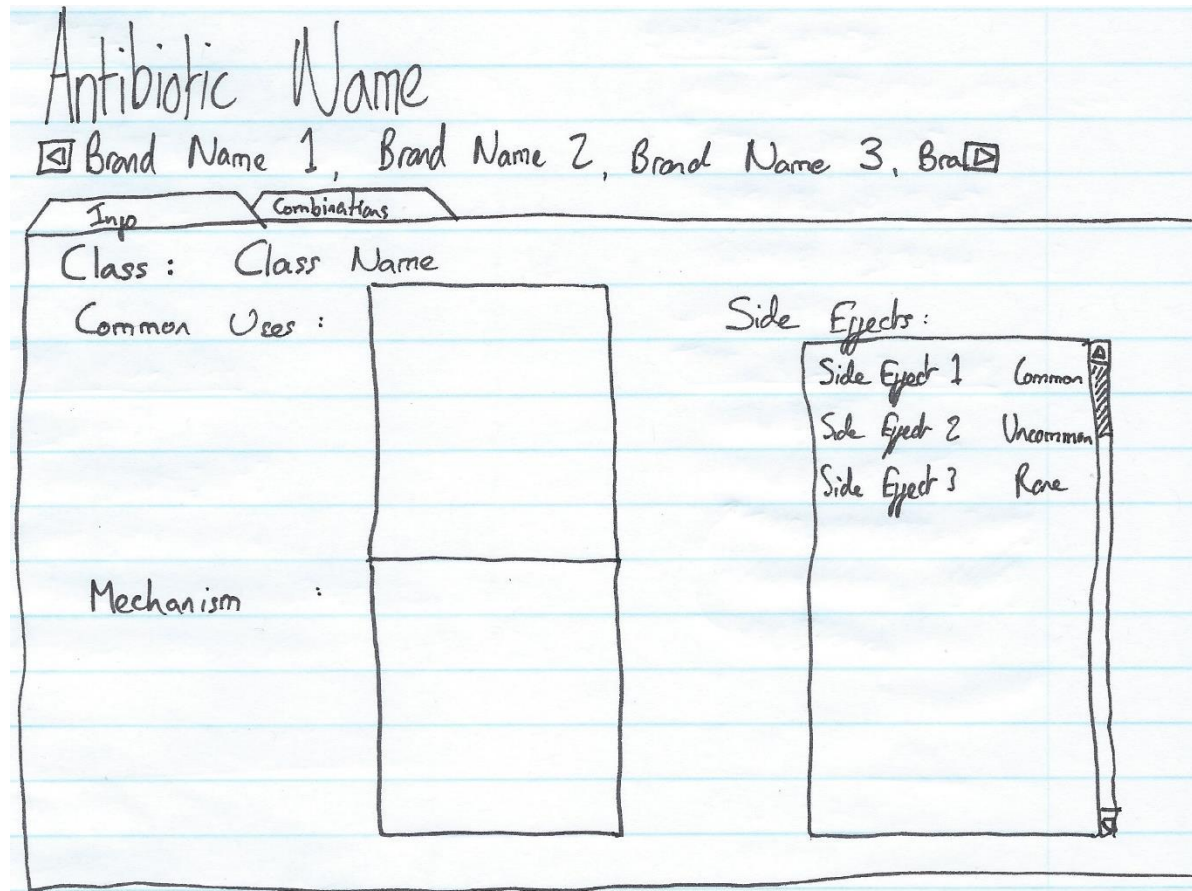
Combination Name

Antibiotic 1	50%
Antibiotic 2	30%
Antibiotic 3	20%

Study 1
Study 2

Treatments

Study Name

Bacterial Species: Species Name

Isolates:

All	
Isolate 1	Source
Isolate 2	Source
Isolate 3	Source

FIC:

All
$0.5\times$
$1.0\times$
$2.0\times$
$4.0\times$
$8.0\times$

Results:

20 minutes	80%
40 minutes	72%
60 minutes	60%
120 minutes	40%

Graph:

Appendix 3: Screenshots of Databank Viewing Screens

Antibiotics Data Bank
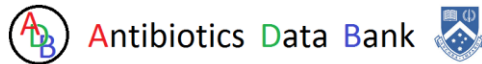
| Antibiotics | Classes | Combinations | Studies |

List of Antibiotics

By Name

Amikacin
Amoxicillin
Ampicillin
Arsphenamine
Azithromycin
Azlocillin
Aztreonam
Bacitracin
Benzylpenicillin
Capreomycin
Carbenicillin
Cefaclor
Cefadroxil
Cefalexin
Cefalotin
Cefamandole
Cefazolin
Cefdinir
Cefditoren
Cefepime
Cefixime
Cefoperazone
Cefotaxime
Cefoxitin
Cefpodoxime
Cefprozil
Ceftaroline Fosamil
Ceftazidime
Ceftibuten
Ceftizoxime
Ceftobiprole
Ceftriaxone
Cefuroxime
Chloramphenicol
Cilastatin
Ciprofloxacin
Clarithromycin
Clindamycin
Clofazimine
Cloxacillin
Colistin
Cycloserine
Dalfopristin
Dapsone
Daptomycin
Demeclocycline

Dicloxacillin
Dirithromycin
Doripenem
Doxycycline
Enoxacin
Ertapenem
Erythromycin
Ethambutol
Ethionamide
Flucloxacillin
Fosfomycin
Furazolidone
Fusidic Acid
Gatifloxacin
Geldanamycin
Gemifloxacin
Gentamicin
Grepafloxacin
Herbimycin
Imipenem
Isoniazid
Kanamycin
Levofloxacin
Lincomycin
Linezolid
Lomefloxacin
Loracarbef
Mafenide
Meropenem
Methicillin
Metronidazole
Mezlocillin
Minocycline
Moxifloxacin
Mupirocin
Nafcillin
Nalidixic Acid
Neomycin
Netilmicin
Nitrofurantoin
Norfloxacin
Ofloxacin
Oxacillin
Oxytetracycline
Paromomycin
Phenoxymethylpenicillin

Piperacillin
Platensimycin
Polymyxin B
Posizolid
Pyrazinamide
Quinupristin
Radezolid
Rifabutin
Rifampicin
Rifapentine
Rifaximin
Roxithromycin
Silver Sulfadiazine
Sparfloxacin
Spectinomycin
Spiramycin
Streptomycin
Streptomycin
Sulfacetamide
Sulfadiazine
Sulfadimethoxine
Sulfafurazole
Sulfamethizole
Sulfamethoxazole
Sulfanilimide
Sulfasalazine
Sulfonamidochrysoidine
Tedizolid
Teicoplanin
Telavancin
Telithromycin
Temafloxacin
Temocillin
Tetracycline
Thiamphenicol
Ticarcillin
Tigecycline
Tinidazole
Tobramycin
Trimethoprim
Trimethoprim
Troleandomycin
Trovafloxacin
Vancomycin

By Class

Aminoglycosides
Amikacin
Gentamicin
Kanamycin
Neomycin
Netilmicin
Paromomycin
Spectinomycin
Streptomycin
Tobramycin

Ansamycins
Geldanamycin
Herbimycin
Rifaximin

Carbacephem
Loracarbef

Carbapenems
Cilastatin
Doripenem
Ertapenem
Imipenem
Meropenem

Cephalosporins (Generation 1)
Cefadroxil
Cefalexin
Cefalotin
Cefazolin

Cephalosporins (Generation 2)
Cefaclor
Cefamandole
Cefoxitin
Cefprozil
Cefuroxime

Cephalosporins (Generation 3)
Cefdinir
Cefditoren
Cefixime
Cefoperazone
Cefotaxime
Cefpodoxime
Ceftazidime
Ceftibuten
Ceftizoxime
Ceftriaxone

Cephalosporins (Generation 4)
Cefepime

Cephalosporins (Generation 5)
Ceftaroline Fosamil
Ceftobiprole

Glycopeptides
Teicoplanin
Telavancin
Vancomycin

Lincosamides (Bs)
Clindamycin
Lincomycin

Lipopeptide
Daptomycin

Macrolides (Bs)
Azithromycin
Clarithromycin
Dirithromycin
Erythromycin
Roxithromycin
Spiramycin
Telithromycin
Troleandomycin

Monobactams
Aztreonam

Nitrofurans
Furazolidone
Nitrofurantoin

Others
Arsphenamine
Capreomycin
Chloramphenicol
Clofazimine
Cycloserine
Dalfopristin
Dapsone
Ethambutol
Ethionamide
Fosfomycin
Fusidic Acid
Isoniazid
Metronidazole
Mupirocin
Platensimycin
Pyrazinamide
Quinupristin
Rifabutin
Rifampicin
Rifapentine
Streptomycin
Thiamphenicol
Tigecycline
Tinidazole
Trimethoprim

Oxazolidinones (Bs)
Linezolid
Posizolid
Radezolid
Tedizolid

Penicillins
Amoxicillin
Ampicillin
Azlocillin
Benzylpenicillin
Carbenicillin
Cloxacillin
Dicloxacillin
Flucloxacillin
Methicillin
Mezlocillin
Nafcillin
Oxacillin
Phenoxymethylpenicillin
Piperacillin
Temocillin
Ticarcillin

Polypeptides
Bacitracin
Colistin
Polymyxin B

Quinolones
Ciprofloxacin
Enoxacin
Gatifloxacin
Gemifloxacin
Grepafloxacin
Levofloxacin
Lomefloxacin
Moxifloxacin
Nalidixic Acid
Norfloxacin
Ofloxacin
Sparfloxacin
Temafloxacin
Trovafloxacin

Sulfonamides (Bs)
Mafenide
Silver Sulfadiazine
Sulfacetamide
Sulfadiazine
Sulfadimethoxine
Sulfafurazole
Sulfamethizole
Sulfamethoxazole
Sulfanilimide
Sulfasalazine
Sulfonamidochrysoidine
Trimethoprim

Tetracyclines (Bs)
Demeclocycline
Doxycycline
Minocycline
Oxytetracycline
Tetracycline

Disclaimer goes here

Antibiotics Data Bank

Antibiotics	Classes	Combinations	Studies

Herbimycin ↵   Directory   ↳ Isoniazid

Imipenem

Info	Technical Details	Combinations

Class: Carbapenems

Wikipedia: Imipenem

Common Uses:

Mechanisms:

Side Effects:

Allergic reactions	Common
Diarrhoea	Common
Gastrointestinal upset	Common
Headache	Common
Nausea	Common
Rash	Common
Seizures	Common
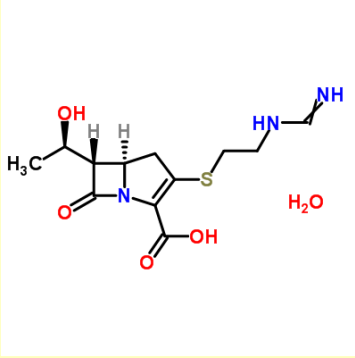
Image generated by ChemSpider.com

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Antibiotics Data Bank

Antibiotics	Classes	Combinations	Studies

Herbimycin ↵   Directory   ↳ Isoniazid

Imipenem

Info	Technical Details	Combinations

CAS Number:	74431-23-5	*ChemSpider ID:*	4445535	*PubChem ID:*	5282372	*Formula:*	$C_{12}H_{17}N_3O_4S$
DrugBank ID:	01598	*KEGG:*		*Molecular Mass:*	299.347	*UNII:*	71OTZ9ZE0A
ChEBI:	51799	*ChEMBL:*	43708	*IUPHAR Ligand:*		*ATC Codes*	J01DH51

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Antibiotics Data Bank

Antibiotics	Classes	Combinations	Studies

Herbimycin ↵   Directory   ↳ Isoniazid

Imipenem

Info	Technical Details	Combinations

Combinations:	Imipenem/Cilastatin ⊃	Antibiotics:		
		Cilastatin	50%
		Imipenem	50%

Disclaimer goes here

Antibiotics Data Bank

Antibiotics	Classes	Combinations	Studies

List of Classes

By Name

Aminoglycosides	Cephalosporins (Generation 5)	Oxazolidinones (Bs)
Ansamycins	Glycopeptides	Penicillins
Carbacephem	Lincosamides (Bs)	Polypeptides
Carbapenems	Lipopeptide	Quinolones
Cephalosporins (Generation 1)	Macrolides (Bs)	Sulfonamides (Bs)
Cephalosporins (Generation 2)	Monobactams	Tetracyclines (Bs)
Cephalosporins (Generation 3)	Nitrofurans	
Cephalosporins (Generation 4)	Others	

Disclaimer goes here

Antibiotics Data Bank

Antibiotics	Classes	Combinations	Studies

↵   Directory   ↳ Ansamycins

Aminoglycosides

Info	Technical Details	Antibiotics

Wikipedia:	
Common Uses:	
Mechanisms:	

Side Effects:	Hearing Loss	Common
	Kidney Damage	Common
	Vertigo	Common

Disclaimer goes here

Antibiotics Data Bank

| Antibiotics | Classes | Combinations | Studies |

↵   Directory   ↳ Ansamycins

Aminoglycosides

| Info | Technical Details | Antibiotics |

Disclaimer goes here

Antibiotics Data Bank

| Antibiotics | Classes | Combinations | Studies |

↵   Directory   ↳ Ansamycins

Aminoglycosides

| Info | Technical Details | Antibiotics |

Antibiotics:
- Amikacin
- Gentamicin
- Kanamycin
- Neomycin
- Netilmicin
- Paromomycin
- Spectinomycin
- Streptomycin
- Tobramycin

Disclaimer goes here

Antibiotics Data Bank

| Antibiotics | Classes | Combinations | Studies |

List of Combinations

By Name

| Amoxicillin/Clavulanate | Imipenem/Cilastatin | Ticarcillin/Clavulanate |
| Ampicillin/Sulbactam | Piperacillin/Tazobactam | Trimethoprim/Sulfamethoxazole |

By Number of Studies

0

| Amoxicillin/Clavulanate | Ampicillin/Sulbactam | Imipenem/Cilastatin |
| Piperacillin/Tazobactam | Ticarcillin/Clavulanate | Trimethoprim/Sulfamethoxazole |

Disclaimer goes here

Antibiotics Data Bank

Antibiotics	Classes	Combinations	Studies

Ampicillin/Sulbactam ↵   Directory   ↪ Piperacillin/Tazobactam

Imipenem/Cilastatin

Info

Antibiotics:	Cilastatin	50%	*Studies:*	
	Imipenem	50%		

Disclaimer goes here

Antibiotics Data Bank

Antibiotics	Classes	Combinations	Studies

List of Studies

By Name

In vitro pharmacodynamics of colistin against Acinetobacter baumannii clinical isolates

Disclaimer goes here

Antibiotics Data Bank

Antibiotics	Classes	Combinations	Studies

↵   Directory   ↳

In vitro pharmacodynamics of colistin against Acinetobacter baumannii clinical isolates

Info

Antibiotic:	Colistin	*PubMed ID:*	17289768

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Appendix 4: Screenshots of Databank Editing Screens

localhost ▸ antibiotics_databank ▸ antibiotics

| Browse | Structure | SQL | Search | Insert | Export | Import | Operations | Tracking |

✔ Showing rows 0 - 29 (~136 total ⓘ , Query took 0.0023 sec)

```
SELECT *
FROM `antibiotics`
LIMIT 0 , 30
```

☐ Profiling [Inline] [Edit] [Explain SQL] [Create PHP Code] [Refresh]

Page number: 1 ▾ > >>

Show : 30 row(s) starting from row # 30 in horizontal ▾ mode and repeat headers after 100 cells

Sort by key: None ▾

+ Options

	ID	NAME	CLASS_ID	CHEMSPIDER_ID	CAS_NUMBER	PUBCHEM_ID	IUPHAR	DRUGBANK_ID	UNII	KEGG	CHEBI	CHEMBL	FORMULA	MOLECULAR_MASS
☐ Edit Copy Delete	1	Amikacin	1	34635	37517-28-5	37768		00479	84319SGC3C		2637	177	C/22\H/43\N/5\O/13\	585.603
☐ Edit Copy Delete	2	Gentamicin	1	390067	1403-66-3	3467	2427	00798	T6Z9V48IKG	D08013	27412	195892	C/21\H/43\N/5\O/7\	477.596
☐ Edit Copy Delete	3	Kanamycin	1	5810	59-01-8	6032		01172	RUC37XUP2P		17630	1384	C/18\H/36\N/4\O/11\	484.499
☐ Edit Copy Delete	4	Neomycin	1	8075	1404-04-2	8378	709	00994	I16QD7X297	D08260	7508	449118	C/23\H/46\N/6\O/13\	616.644
☐ Edit Copy Delete	5	Netilmicin	1	38195	56391-56-1	41859		00955	4O5J85GJJB	D08268		1572	C/21\H/41\N/5\O/7\	475.58
☐ Edit Copy Delete	6	Tobramycin	1	33377	32986-56-4	36294		00684	VZ8RRZ51VK	D00063	28864	1747	C/18\H/37\N/5\O/9\	467.515
☐ Edit Copy Delete	7	Paromomycin	1	390117	1263-89-4	441375		01421			7934	370143	C/23\H/47\N/5\O/18\S	615.629
☐ Edit Copy Delete	8	Streptomycin	1	18508	57-92-1	19649		01082	Y45QSO73OB	D08531	17076	1201194	C/21\H/39\N/7\O/12\	581.574
☐ Edit Copy Delete	9	Spectinomycin	1	14785	1695-77-8	15541		00919	93AKI1U6QF	D08526	9215	1167	C/14\H/24\N/2\O/7\	332.35
☐ Edit Copy Delete	10	Geldanamycin	2	10272739	30562-34-6			02424				278315	C/29\H/40\N/2\O/9\	560.64
☐ Edit Copy Delete	11	Herbimycin	2	10272738	70563-58-5	6436247						1159659	C/30\H/42\N/2\O/9\	574.66
☐ Edit Copy Delete	12	Rifaximin	2	10482302	80621-81-4	6436173		01220	L36O5T016N	D02554	75246	1617	C/43\H/51\N/3\O/11\	785.879
☐ Edit Copy Delete	13	Loracarbef	3	4447634	76470-66-1	5284584		00447	W72I5ZT78Z	D08143		1013	C/16\H/16\ClN/3\O/4\	349.769
☐ Edit Copy Delete	14	Ertapenem	4	132758	153832-46-3	150610		00303	G32F6EID2H	D04049	404903	1359	C/22\H/25\N/3\O/7\S	475.516
☐ Edit Copy Delete	15	Doripenem	4	66040	148016-81-3	73303			BHV525JOBH	D03895		491571	C/15\H/24\N/4\O/6\S/2\	420.504
☐ Edit Copy Delete	16	Imipenem	4	4445535	74431-23-5	5282372		01598	71OTZ9ZE0A		51799	43708	C/12\H/17\N/3\O/4\S	299.347
☐ Edit Copy Delete	17	Cilastatin	4	4940183	82009-34-5	5280454		01597	141A6AMN38	D07698	3697	766	C/16\H/26\N/2\O/5\S	358.454
☐ Edit Copy Delete	18	Meropenem	4	389924	119478-56-7	441130		00760	FV9J3JU8B1	D02222	43968	127	C/17\H/25\N/3\O/5\S	383.464
☐ Edit Copy Delete	19	Cefadroxil	5	43629	66592-87-8	47964		01140	280111G160	D02353	53667	1644	C/16\H/17\N/3\O/5\S	363.389
☐ Edit Copy Delete	20	Cefazolin	5	30723	25953-19-9	33255		01327	IHS69L0Y4T	D02299	474053	1435	C/14\H/14\N/8\O/4\S\3\	454.51
☐ Edit Copy Delete	21	Cefalotin	5	5802	153-61-7	6024		00456	R72LW146E6	D07635	124991	617	C/16\H/16\N/2\O/6\S/2\	396.44
☐ Edit Copy Delete	22	Cefalexin	5	25541	15686-71-2	2666		00567	5SFF1W6677	D00263	3534	1727	C/16\H/17\N/3\O/4\S	347.39
☐ Edit Copy Delete	23	Cefaclor	6	46260	53994-73-3	51038		00833	3Z6FS3IK0K	D00256		8867	C/15\H/14\ClN/3\O/4\S	367.808
☐ Edit Copy Delete	24	Cefamandole	6	401748	34444-01-4	456255		01326	5CKP8C2LLI	D02344	3480	1146	C/18\H/18\N/6\O/5\S/2\	462.505
☐ Edit Copy Delete	25	Cefoxitin	6	389981	35607-66-0	441199		01331	6OEV9DX57Y	D02345	209807	996	C/16\H/17\N/3\O/7\S/2\	427.454
☐ Edit Copy Delete	26	Cefprozil	6	8063315	92665-29-7	9887643		01150	1M698F4H4E	D07651	3506	1742	C/18\H/19\N/3\O/5\S	389.427
☐ Edit Copy Delete	27	Cefuroxime	6	4514699	55268-75-2	5361202		01112	O1R9FJ93ED	D00262		466	C/16\H/16\N/4\O/8\S	424.386
☐ Edit Copy Delete	28	Cefixime	7	4514923										0
☐ Edit Copy Delete	29	Cefdinir	7	5291705										0
☐ Edit Copy Delete	30	Cefditoren	7	8046534										0

↑ Check All / Uncheck All With selected: ✏ Change ⊘ Delete Export

Page number: 1 ▾ > >>

Show : 30 row(s) starting from row # 30 in horizontal ▾ mode and repeat headers after 100 cells

Query results operations

🖨 Print view 🖨 Print view (with full texts) Export Display chart Create view

🔖 Bookmark this SQL query

Label: [_____] ☐ Let every user access this bookmark

[Bookmark this SQL query]

Navigation

- Antibiotics
- Classes
- Common Uses
- Mechanisms
- Side Effects
- Likelihoods

Antibiotics

		Name	Brand Name	Class	Common Use	Mechanism	Side Effects and Likelihood	Compendia ID	CAS Number	PubChem ID	EUPHIX	DrugBank ID	UNII	KEGG	CHEBI	CHEMBL	Formula	Molecular Mass	ATC Code
Delete	Update																		

Classes

Common Uses

Mechanisms

Side Effects

Likelihoods