

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 <u>http://en.wikipedia.org/wiki/List_of_antibiotics</u>, 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 #FFFBB, 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 middevelopment 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	Туре	
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)	
СНЕВІ	varchar(60)	
CHEMBL	varchar(60)	
FORMULA	varchar(60)	
MOLECULAR_MASS	float	
Keyname	Column	Unique
ID	ID	Yes
NAME	NAME	Yes
	ID	163
CLASS_ID	CLASS_ID	Yes
	ID	105
antibiotic_atc_codes		
Column	Туре	
ID	int(11)	
ANTIBIOTIC_ID	int(11)	
CODE	varchar(60)	
Keyname	Column	Unique
ID	ID	Yes
ANTIBIOTIC_ID	ANTIBIOTIC_ID	Yes
-	ID	
antibiotic brand names		
antibiotic_brand_names Column	Tuno	
ID	Type	
	int(11)	
ANTIBIOTIC_ID	int(11)	
	varchar(60)	
DISCONTINUED	tinyint(1)	
Keyname	Column	Unique

ID ANTIBIOTIC_ID	ID ANTIBIOTIC_ID ID	Yes Yes
<i>classes</i> Column ID NAME	Type int(11) varchar(60)	
Keyname ID NAME	Column ID NAME	Unique Yes No
<i>combinations</i> Column ID NAME	Type int(11) varchar(150)	
Keyname ID NAME	Column ID NAME ID	Unique Yes Yes
<i>combination_antibiotic_link</i> Column ID COMBINATION_ID ANTIBIOTIC_ID PROPORTION	Type int(11) int(11) int(11) float	
Keyname ID COMBINATION_ID +	Column ID COMBINATION_ID	Unique Yes
ANTIBIOTIC_ID + COMBINATION_ID	ANTIBIOTIC_ID ID ANTIBIOTIC_ID COMBINATION_ID ID	Yes Yes
<i>combination_brand_names</i> Column ID COMBINATION_ID NAME	Type int(11) int(11) varchar(60)	
Keyname	Column	Unique

ID COMBINATION_ID	ID COMBINATION_ID ID	Yes Yes
<i>combination_treatment_link</i> Column ID COMBINATION_ID TREATMENT_ID	Type int(11) int(11) int(11)	
Keyname ID COMBINATION_ID + TREATMENT_ID	Column ID COMBINATION_ID TREATMENT_ID ID	Unique Yes Yes
TREATMENT_ID + COMBINATION_ID	TREATMENT_ID COMBINATION_ID ID	Yes
<i>common_uses</i> Column ID TEXT	Type int(11) varchar(100)	
Keyname ID	Column ID	Unique Yes
•		-
ID common_use_antibiotic_link Column ID ANTIBIOTIC_ID	ID Type int(11) int(11) int(11) Column ID	-
ID common_use_antibiotic_link Column ID ANTIBIOTIC_ID COMMON_USE_ID Keyname	ID Type int(11) int(11) int(11) Column	Yes
ID common_use_antibiotic_link Column ID ANTIBIOTIC_ID COMMON_USE_ID Keyname ID ANTIBIOTIC_ID +	ID Type int(11) int(11) int(11) Column ID ANTIBIOTIC_ID COMMON_USE_ID	Yes Unique Yes

COMMON_USE_ID	int(11)	
Keyname ID	Column ID	Unique 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	Туре	
ID	int(11)	
STUDY_ID	int(11)	
SPECIES_ID	int(11)	
SOURCE	varchar(100)	
Keyname	Column	Unique
ID	ID	Yes
	STUDY_ID	
STUDY_ID + SPECIES_ID	SPECIES_ID	Yes
	ID	
	SPECIES_ID	
SPECIES_ID + STUDY_ID	STUDY_ID	Yes
	ID	
likelihood		
Column	Туре	
ID	int(11)	
NAME	varchar(30)	
Keyname	Column	Unique
ID	ID	Yes
mechanisms		
Column	Туре	
ID	int(11)	
TEXT	varchar(100)	
Keyname	Column	Unique
ID	ID	Yes
mechanism_antibiotic_link		
Column	Туре	
ID	int(11)	

ANTIBIOTIC_ID	int(11)	
MECHANISM_ID	int(11)	
—		
Keyname	Column	Unique
ID	ID	Yes
	ANTIBIOTIC_ID	105
ANTIBIOTIC_ID +	MECHANISM ID	Yes
MECHANISM_ID	—	163
MECHANISM_ID +	MECHANISM_ID	
ANTIBIOTIC_ID	ANTIBIOTIC_ID	Yes
-	ID	
mechanism_class_link		
Column	Туре	
ID	int(11)	
CLASS_ID	int(11)	
MECHANISM_ID	int(11)	
—		
Keyname	Column	Unique
ID	ID	Yes
	CLASS_ID	
CLASS_ID + MECHANISM_ID	MECHANISM_ID	Yes
	—	163
	ID	
	MECHANISM_ID	
MECHANISM_ID + CLASS_ID	_	Yes
MECHANISM_ID + CLASS_ID	CLASS_ID	Yes
MECHANISM_ID + CLASS_ID	_	Yes
	CLASS_ID	Yes
side_effects	CLASS_ID ID	Yes
side_effects Column	CLASS_ID ID Type	Yes
side_effects	CLASS_ID ID	Yes
side_effects Column	CLASS_ID ID Type	Yes
side_effects Column ID	CLASS_ID ID Type int(11)	Yes
side_effects Column ID	CLASS_ID ID Type int(11)	Yes Unique
side_effects Column ID TEXT	CLASS_ID ID Type int(11) text	
side_effects Column ID TEXT Keyname	CLASS_ID ID Type int(11) text Column	Unique
side_effects Column ID TEXT Keyname	CLASS_ID ID Type int(11) text Column	Unique
side_effects Column ID TEXT Keyname ID	CLASS_ID ID Type int(11) text Column	Unique
side_effects Column ID TEXT Keyname ID side_effect_antibiotic_link	CLASS_ID ID Type int(11) text Column ID	Unique
side_effects Column ID TEXT Keyname ID side_effect_antibiotic_link Column ID	CLASS_ID ID Type int(11) text Column ID Type int(11)	Unique
side_effects Column ID TEXT Keyname ID side_effect_antibiotic_link Column ID ANTIBIOTIC_ID	CLASS_ID ID Type int(11) text Column ID Type int(11) int(11)	Unique
side_effects Column ID TEXT Keyname ID side_effect_antibiotic_link Column ID ANTIBIOTIC_ID SIDE_EFFECT_ID	CLASS_ID ID Type int(11) text Column ID Type int(11) int(11) int(11)	Unique
side_effects Column ID TEXT Keyname ID side_effect_antibiotic_link Column ID ANTIBIOTIC_ID	CLASS_ID ID Type int(11) text Column ID Type int(11) int(11)	Unique
side_effects Column ID TEXT Keyname ID side_effect_antibiotic_link Column ID ANTIBIOTIC_ID SIDE_EFFECT_ID LIKELIHOOD_ID	CLASS_ID ID Type int(11) text Column ID Type int(11) int(11) int(11) int(11)	Unique Yes
side_effects Column ID TEXT Keyname ID side_effect_antibiotic_link Column ID ANTIBIOTIC_ID SIDE_EFFECT_ID LIKELIHOOD_ID Keyname	CLASS_ID ID Type int(11) text Column ID Type int(11) int(11) int(11) int(11) int(11)	Unique Yes
side_effects Column ID TEXT Keyname ID side_effect_antibiotic_link Column ID ANTIBIOTIC_ID SIDE_EFFECT_ID LIKELIHOOD_ID	CLASS_ID ID Type int(11) text Column ID Type int(11) int(11) int(11) int(11)	Unique Yes

ANTIBIOTIC_ID + SIDE_EFFECT_ID SIDE_EFFECT_ID + ANTIBIOTIC_ID	SIDE_EFFECT_ID ID SIDE_EFFECT_ID ANTIBIOTIC_ID ID	Yes
side_effect_class_link Column ID CLASS_ID SIDE_EFFECT_ID LIKELIHOOD_ID	Type int(11) int(11) int(11) int(11)	
Keyname ID	Column ID CLASS_ID	Unique Yes
CLASS_ID + SIDE_EFFECT_ID	SIDE_EFFECT_ID	Yes
SIDE_EFFECT_ID + CLASS_ID	SIDE_EFFECT_ID CLASS_ID ID	Yes
species Column ID NAME Keyname ID	Type int(11) varchar(60) Column ID	Unique Yes
study Column ID ENTITY_ID ENTITY_TYPE PUBMED_ID NAME	Type int(11) int(11) varchar(1) int(11) varchar(100)	
Keyname ID NAME ENTITY_ID + NAME	Column ID NAME ID ENTITY_ID NAME ID	Unique Yes Yes Yes

<i>time_kill_series</i> Column ID ISOLATE_ID FIC TIME_MIN CONCENTRATION	Type int(11) int(11) double int(11) double	
Keyname ID	Column ID ISOLATE_ID	Unique Yes
ISOLATE_ID + FIC + CONCENTRATION + TIME_MIN	FIC CONCENTRATION TIME_MIN ID	Yes
treatments		
Column	Туре	
ID	int(11)	
NAME	varchar(60)	
Keyname ID	Column ID	Unique Yes
urls		
<i>urls</i> Column	Туре	
	Type varchar(100)	
Column		
Column CHEMSPIDER_IMAGE_START	varchar(100)	
Column CHEMSPIDER_IMAGE_START CHEMSPIDER_IMAGE_END	varchar(100) varchar(100)	
Column CHEMSPIDER_IMAGE_START CHEMSPIDER_IMAGE_END CAS_NUMBER_START	varchar(100) varchar(100) varchar(100)	
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Column CHEMSPIDER_IMAGE_START CHEMSPIDER_IMAGE_END CAS_NUMBER_START CAS_NUMBER_END PUBCHEM_ID_START PUBCHEM_ID_END DRUGBANK_ID_END DRUGBANK_ID_END KEGG_START KEGG_END UNII_START UNII_END CHEBI_START CHEBI_END CHEMBL_END	varchar(100) varchar(100) varchar(100) varchar(100) varchar(100) varchar(100) varchar(100) varchar(100) varchar(100) varchar(100) varchar(100) varchar(100) varchar(100) varchar(100) varchar(100)	
Column CHEMSPIDER_IMAGE_START CHEMSPIDER_IMAGE_END CAS_NUMBER_START CAS_NUMBER_END PUBCHEM_ID_START PUBCHEM_ID_END DRUGBANK_ID_START DRUGBANK_ID_START DRUGBANK_ID_END KEGG_START KEGG_END UNII_START UNII_END CHEBI_START CHEBI_END CHEMBL_START CHEMBL_END IUPHAR_START	varchar(100) varchar(100) varchar(100) varchar(100) varchar(100) varchar(100) varchar(100) varchar(100) varchar(100) varchar(100) varchar(100) varchar(100) varchar(100) varchar(100) varchar(100) varchar(100)	
Column CHEMSPIDER_IMAGE_START CHEMSPIDER_IMAGE_END CAS_NUMBER_START CAS_NUMBER_END PUBCHEM_ID_START PUBCHEM_ID_END DRUGBANK_ID_END DRUGBANK_ID_END KEGG_START KEGG_END UNII_START UNII_END CHEBI_START CHEBI_END CHEMBL_END	varchar(100) varchar(100) varchar(100) varchar(100) varchar(100) varchar(100) varchar(100) varchar(100) varchar(100) varchar(100) varchar(100) varchar(100) varchar(100) varchar(100) varchar(100)	
Column CHEMSPIDER_IMAGE_START CHEMSPIDER_IMAGE_END CAS_NUMBER_START CAS_NUMBER_END PUBCHEM_ID_START PUBCHEM_ID_END DRUGBANK_ID_START DRUGBANK_ID_END KEGG_START KEGG_END UNII_START UNII_END CHEBI_START CHEBI_END CHEMBL_START CHEMBL_END IUPHAR_START IUPHAR_END	varchar(100) varchar(100) varchar(100) varchar(100) varchar(100) varchar(100) varchar(100) varchar(100) varchar(100) varchar(100) varchar(100) varchar(100) varchar(100) varchar(100) varchar(100) varchar(100) 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

Antibiotic Wame	
Brand Name 1, Brand Name Z, Brand Name 3, Brand	
Ingo Combinations	
Class: Class Name	
Common Uses: Side Eyects:	-
Side Eyect 1 Common Sole Eyect 2 Uncommon	9
Sole Eyect 2 Uncommu	A
Side Eyect 3 Rore	
Mechanism	1
	ति
Injo Compinations	
Combination 1 Autobic 1 50%	
Combination 2 Antibiotic Z 30%	

Combination Name Treatments Antibiotic 1 50% Study 1 Number of Street Antibiohic Z 30% Study 2 Antibiotic 3 20% Study Name Bacterial Species : Species Name Isolates: FIC : All All The second s Isolate 1 Source 0.5 * Isolate 2 1.0 + Source Isolale 3 Source 2.0x 4.0% 8.0× Groph : Results : 100 20 minutes 80% 80 40 minuter 72% 60 60 minutes 60% 40 120 minutes 40% 20

Appendix 3: Screenshots of Databank Viewing Screens

Antibiotics	Data Bank 🐰	2
Antibiotics Classes Combination	ss Studies	
By Name		
Amikacin Amoxicillin	Dicloxacillin Dirithromycin	<u>Piperacillin</u> <u>Platensimycin</u>
Ampicillin Arsphenamine	Doripenem Doxycycline	Polymyxin B Posizolid
Azithromycin	Enoxacin	Pyrazinamide
Azlocillin Aztreonam	Ertapenem Ervthromycin	Quinupristin Radezolid
Bacitracin	Ethambutol Ethionamide	Rifabutin
Benzylpenicillin Capreomycin	Flucloxacillin	Rifapentine
Carbenicillin Cefaclor	Fosfomycin Furazolidone	<u>Rifaximin</u> Roxithromycin
Cefadroxi1 Cefalexin	Fusidic Acid Gatifloxacin	Silver Sulfadiazine Sparfloxacin
Cefalotin	Geldanamycin	Spectinomycin
Cefamandole Cefazolin	Gemifloxacin Gentamicin	Spiramycin Streptomycin
Cefdinir	Grepafloxacin	Streptomycin
Cefditoren Cefepime	Herbimycin Imipenem	<u>Sulfacetamide</u> <u>Sulfadiazine</u>
Cefixime Cefoperazone	Isoniazid Kanamycin	Sulfadimethoxine Sulfafurazole
Cefotaxime Cefoxitin	Levofloxacin Lincomycin	Sulfamethizole Sulfamethoxazole
Cefpodoxime	Linezolid	Sulfanilimide
Cefprozil Ceftaroline Fosamil	Lomefloxacin Loracarbef	Sulfasalazine Sulfonamidochrysoidine
Ceftazidime	Mafenide	Tedizolid
Ceftibuten Ceftizoxime	Meropenem Methicillin	Teicoplanin Telavancin
Ceftobiprole Ceftriaxone	Metronidazole Mezlocillin	<u>Telithromycin</u> Temafloxacin
Cefuroxime	Minocycline	Temocillin
Chloramphenicol <u>Cilastatin</u>	Moxifloxacin Mupirocin	Tetracycline Thiamphenicol
Ciprofloxacin Clarithromycin	Nafcillin Nalidixic Acid	Ticarcillin Tigecycline
Clindamycin	Neomycin	Tinidazole
Clofazimine Cloxacillin	Netilmicin Nitrofurantoin	Tobramycin Trimethoprim
Colistin Cvcloserine	Norfloxacin Ofloxacin	Trimethoprim Troleandomycin
Dalfopristin	Oxacillin	Trovafloxacin
Daptomycin	Oxvtetracvcline Paromomycin	Vancomvein
Demeclocycline	Phenoxymethylpenicillin	
By Class		
Aminoglycosides Amikacin	Lincosamides (Bs) Clindamycin	Polypeptides Bacitracin
Gentamicin Kanamycin	Linconvein	Colistin Polymyxin B
Neomycin	Lipopeptide	
<u>Netilmicin</u> Paromomycin	Daptomycin	Quinolones Ciprofloxacin
Spectinomycin	Macrolides (Bs) Azithromycin	Enoxacin Gatifloxacin
Streptomycin Tobramycin	Clarithromycin	Gemifloxacin
Ansamycins	Dirithromycin Erythromycin	Grepafloxacin Levofloxacin
Geldanamycin	Roxithromycin	Lomefloxacin
Herbimycin Rifaximin	Spiramycin Telithromycin	<u>Moxifloxacin</u> <u>Nalidixic Acid</u>
Carbacephem	Troleandomycin	<u>Norfloxacin</u> Ofloxacin
Loracarbef	Monobactams	Sparfloxacin
Carbapenems	Aztreonam	<u>Temafloxacin</u> <u>Trovafloxacin</u>
Cilastatin Doripenem	Nitrofurans Furazolidone	Sulfonamides (Bs)
Ertapenem	Nitrofurantoin	Mafenide
Imipenem Meropenem	Others	Silver Sulfadiazine Sulfacetamide
Cephalosporins (Generation 1)	Arsphenamine Capreomycin	Sulfadinzine Sulfadimethoxine
Cefadroxil	Chloramphenicol	Sulfafurazole
Cefalexin Cefalotin	Clofazimine Cycloserine	Sulfamethizole Sulfamethoxazole
Cefazolin	Dalfopristin Dapsone	Sulfanilimide Sulfasalazine
Cephalosporins (Generation 2)	Ethambutol	Sulfonamidochrysoidine
Cefaclor Cefamandole	Ethionamide Fosfomvcin	Trimethoprim
<u>Cefoxitin</u> <u>Cefprozil</u>	Fusidic Acid Isoniazid	Tetracyclines (Bs) Demeclocycline
Cefuroxime	Metronidazole Mupirocin	Doxycycline Minocycline
Cephalosporins (Generation 3)	Platensimycin	Oxytetracycline
Cefdinir Cefditoren	Pyrazinamide Quinupristin	Tetracycline
Cefixime Cefoperazone	Rifabutin	
Cefotaxime	Rifampicin Rifapentine	
Cefpodoxime Ceftazidime	Streptomycin Thiamphenicol	
Ceftibuten	Tigecycline	
Ceftizoxime Ceftriaxone	Tinidazole Trimethoprim	
Cephalosporins (Generation 4)	Oxazolidinones (Bs)	
Cefepime	Linezolid Posizolid	
Cephalosporins (Generation 5)	Radezolid	
Ceftaroline Fosamil Ceftobiprole	Tedizolid	
Glycopeptides	Penicillins Amoxicillin	
Teicoplanin	Ampicillin	
<u>Telavancin</u> Vancomycin	Azlocillin Benzylpenicillin	
	Carbenicillin Cloxacillin	
	Dicloxacillin	
	Flucloxacillin Methicillin	
	Mezlocillin Nafcillin	
	Oxacillin	
	Phenoxymethylpenicillin Piperacillin	
	Temocillin Ticarcillin	
	Insultini	
Disclaimer goes here		

	Antibio	otics	Data E	Ban	ık 🌄	
Antibiotics	<u>Classes</u>	Combinations	Studies			
Imipene	m		<u>Herbimycin</u> ↔	<u>Direct</u>	tory 🗘 Isoniazid	
Info	Technical Details	Combinations				
Class:	Carbapenems		Wikipedia:	Imipenem		
Common Uses:						
Mechanisms:						
Side Effects:	Allergic reactions	Common				
	Diarrhoea	Common	-		ŇH	
	Gastrointestinal upset	Common	_			
	Headache	Common			H ₃ C	
	Nausea	Common			¹¹ ³ ³	
	Rash	Common			H ₂ O	
	Seizures	Common			V (
					он с	
					Image generated by <u>ChemSpiden.com</u>	

	Antibi	otics	Data	Bank			
Antibiotics	Classes	Combinations	Studies				
			<u>Herbimycin</u> ح	Directory	↔ <u>Isoniazid</u>		
Imipene	m						
Info	Technical Details	Combinations					
CAS Number:	<u>74431-23-5</u>	ChemSpider ID:	<u>4445535</u>	PubChem ID:	<u>5282372</u>	Formula:	$C_{12}H_{17}N_{3}O_{4}S$
DrugBank ID:	<u>01598</u>	KEGG:		Molecular Mass:	299.347	UNII:	71OTZ9ZE0A
ChEBI:	<u>51799</u>	ChEMBL:	<u>43708</u>	IUPHAR Ligand:		ATC Codes	<u>J01DH51</u>

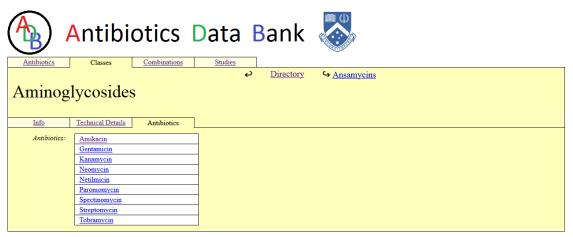
	<mark>A</mark> ntibi	otics I	Data I	Bank		
Antibiotics	<u>Classes</u>	Combinations	Studies			
			Herbimycin 🕹	Directory	↔ <u>Isoniazid</u>	
Imipen						
Info	Technical Details	Combinations				
Combinatio	ns: Imipenem/Cilas	statin	Antibiotics:	<u>Cilastatin</u> Imipenem	50% 50%	

Antibiotics	Data Bank 🐺	
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	

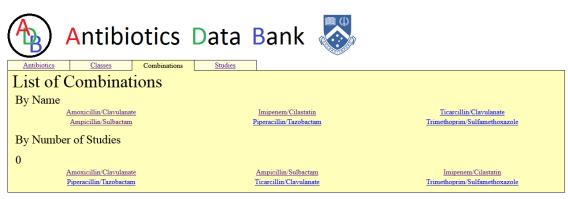
Disclaimer goes here

	Antibi	otics	Data	Bank	
Antibiotics	Classes	Combinations	Studies		
			ب	Directory	↔ <u>Ansamycins</u>
Aminog	lycosides	5			
Info	Technical Details	Antibiotics]		
Wikipedia:					
Common Uses:					
Mechanisms:					
Side Effects:	Hearing Loss	Common			
	Kidney Damage	Common	1		
	Vertigo	Common			





Disclaimer goes here



	Antibio	otics	Data I	Bank	
Antibiotics	Classes	Combinations	Studies		
		Ampici	llin/Sulbactam +	Directory	↔ Piperacillin/Tazobactam
Imipene	m/Cilasta	atin			
Antibiotics:	<u>Cilastatin</u> <u>Imipenem</u>	50% 50%	Studies:		



	Antibiotics	Data E	Bank	
Antibiotics	Classes Combinations	Studies		
		ب	Directory	с ,
In vitro	pharmacodynam	nics of colis	stin agai	nst Acinetobacter baumannii
clinical	isolates			
Info	1			
Antibiotic:	Colistin	PubMed ID:	<u>17289768</u>	

Appendix 4: Screenshots of Databank Editing Screens

🗊 localhost 🕨 🗊 antibiotics_dat	abank							
M Structure D SQL	Search 🗐 Query	Export 📑 Ir	nport 🥜	Operations	💻 Privile	ges 💿 Tracking	de Desig	gner
Table 🔪	Action			Rows	😡 Туре	Collation	Size	Overhead
antibiotics	🔲 Browse 🥻 Structur	e 🤹 Search 📑 Insert	🗒 Empty 🌾	Drop	136 InnoDB	latin1_swedish_ci	48.0 KiB	-
antibiotic_atc_codes	🔲 Browse 🥻 Structur	e 🤹 Search 📑 Insert	🗄 Empty 🌾	Drop	55 InnoDB	latin1_swedish_ci	32.0 KiB	-
antibiotic_brand_names	🔲 Browse 🥖 Structur	e 🧟 Search 👫 Insert	🗒 Empty 🄇	Drop	138 InnoDB	latin1_swedish_ci	32.0 KiB	-
Classes	🔲 Browse 🥻 Structur	e 🤹 Search 😼 Insert	🗒 Empty 🔇	Drop	²² InnoDB	latin1_swedish_ci	32.0 KiB	-
combinations	🔲 Browse 🥻 Structur	e 🤹 Search 👫 Insert	🗒 Empty 🌾	Drop	⁶ InnoDB	latin1_swedish_ci	32.0 KiB	-
combination_antibiotic_link	🔲 Browse 🥻 Structur	e 🤹 Search 👫 Insert	🗒 Empty 🌾	Drop	² InnoDB	latin1_swedish_ci	48.0 KiB	-
combination_brand_names	🔟 Browse 🥖 Structur	e 🧟 Search 👫 Insert	🗒 Empty 🔇	Drop	⁸ InnoDB	latin1_swedish_ci	32.0 KiB	-
combination_treatment_link	🔲 Browse 🥻 Structur	e 🔛 Search 😼 Insert	🖀 Empty 🔇	Drop	⁰ InnoDB	latin1_swedish_ci	48.0 KiB	-
common_uses	🔲 Browse 🥻 Structur	e 😰 Search 👫 Insert	🖀 Empty 🔇	Drop	⁰ InnoDB	latin1_swedish_ci	16.0 KiB	-
common_use_antibiotic_link	🗉 Browse 📝 Structur	e 🔝 Search 📑 Insert	🖀 Empty 🔇	Drop	⁰ InnoDB	latin1_swedish_ci	48.0 KiB	-
common_use_class_link	🔲 Browse 📝 Structur	e 🔝 Search 📑 Insert	🖀 Empty 🄇	Drop	⁰ InnoDB	latin1_swedish_ci	48.0 KiB	-
isolates	🔲 Browse 🥻 Structur	e 🤹 Search 👫 Insert	🗒 Empty 🔇	Drop	⁵ InnoDB	latin1_swedish_ci	48.0 KiB	-
likelihood	🔲 Browse 🥖 Structur	e 🤹 Search 👫 Insert	🗄 Empty 🄇	Drop	7 InnoDB	latin1_swedish_ci	16.0 KiB	-
mechanisms	🔲 Browse 🥻 Structur	e 😰 Search 👫 Insert	🖀 Empty 🔇	Drop	⁰ InnoDB	latin1_swedish_ci	16.0 KiB	-
mechanism_antibiotic_link	🔳 Browse 📝 Structur	e 🔛 Search 📑 Insert	🖀 Empty 🄇	Drop	⁰ InnoDB	latin1_swedish_ci	48.0 KiB	-
mechanism_class_link	🔲 Browse 🥻 Structur	e 🔛 Search 📑 Insert	🖀 Empty 🔇	Drop	⁰ InnoDB	latin1_swedish_ci	48.0 KiB	-
side_effects	🔲 Browse 📝 Structur	e 🤹 Search 👫 Insert	🗒 Empty 🄇	Drop	38 InnoDB	latin1_swedish_ci	16.0 KiB	-
side_effect_antibiotic_link	🔲 Browse 🥻 Structur	e 🤹 Search 👫 Insert	🗄 Empty 🌾	Drop	¹⁴⁸ InnoDB	latin1_swedish_ci	48.0 KiB	-
side_effect_class_link	🔲 Browse 🥻 Structur	e 🤏 Search 👫 Insert	🗄 Empty 🄇	Drop	³⁰ InnoDB	latin1_swedish_ci	48.0 KiB	-
species	🔲 Browse 🥻 Structur	e 🤹 Search 👫 Insert	🗒 Empty 🔇	Drop	¹ InnoDB	latin1_swedish_ci	16.0 KiB	-
study	🔲 Browse 屋 Structur	e 🤹 Search 📑 Insert	🗄 Empty 🄇	Drop	¹ InnoDB	latin1_swedish_ci	48.0 KiB	-
time_kill_series	🔲 Browse 🥻 Structur	e 😰 Search 📑 Insert	🖀 Empty 🔇	Drop	⁰ InnoDB	latin1_swedish_ci	32.0 KiB	-
treatments	🔲 Browse 📝 Structur	e 🔝 Search 📑 Insert	🖀 Empty 🄇	Drop	⁰ InnoDB	latin1_swedish_ci	16.0 KiB	-
urls	🔲 Browse 🥻 Structur	e 🤹 Search 📑 Insert	🗄 Empty 🌾	Drop	¹ InnoDB	latin1_swedish_ci	16.0 KiB	-
24 tables	Sum				⁵⁹⁸ InnoDB	latin1_swedish_ci	832.0 KiB	0 B
Check All / Uncheck All	With selected: 👻							

🚔 Print view 👼 Data Dictionary

Treate table on database antibiotics_databank
Name: Number of columns:
Go

27

🗐 localhost 🖡 🕡 antibiotics_databank 🖡 🐻 antibio 🗏 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 v > >> Show : 30 row(s) starting from row # 30 in horizontal v mode and repeat headers after 100 cells Sort by key: None ~ . ←⊤→ ID NAME CLASS_ID CHEMSPIDER_ID CAS_NUMBER PUBCHEM_ID IUPHAR DRUGBANK_ID UNII KEGG CHEBI CHEMBL FORMULA MOLECULAR_MASS 🗌 🥒 Edit 賭 Copy 🤤 Delete 1 Amikacin 1 34635 37517-28-5 37768 00479 84319SGC3C 2637 177 585.603 C/22\H 🔲 🥜 Edit 👫 Copy 🤤 Delete 2 Gentamicin C/21\H /43\N/5\O/7\ 1 390067 1403-66-3 3467 00798 T6Z9V48IKG D08013 27412 195892 477.596 2427 🗌 🥜 Edit 👫 Copy 🥥 Delete 3 Kanamycin 1 5810 59-01-8 6032 01172 RUC37XUP2P 17630 1384 C/18\H /36\N/4 484.499 🗌 🖉 Edit 🔆 Copy 😂 Delete 4 Neomycin 1 8075 1404-04-2 8378 709 00994 I16QD7X297 D08260 7508 449118 C/23\H 616.644 🗌 🥜 Edit 👫 Copy 😑 Delete 5 Netilmicin 1 38195 56391-56-1 41859 405J85GJJB D08268 475.58 00955 1572 C/21\H /41\N/5\O/7\ 🗌 🥔 Edit 👫 Copy 🤤 Delete 6 Tobramycin 1 33377 VZ8RRZ51VK D00063 28864 1747 467.515 32986-56-4 36294 00684 C/18\H /37\N/5\O/9 C/23\H /47\N/5 \O/18\S 📋 🖉 Edit 👫 Copy 🥥 Delete 7 Paromomycin 1 390117 1263-89-4 441375 01421 7934 370143 615.629 Y45QSO73OB D08531 17076 1201194 C/21VH 1 18508 📄 🥜 Edit 👫 Copy 🤤 Delete 🛛 8 Streptomycin 57-92-1 19649 01082 581.574 /39\N/7 \O/12\ 🗌 🥜 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 Copy Colete 11 Herbimycin 2 10272738 70563-58-5 6436247 1159659 C/30\H /42\N/2\O/9\ 574.66 🗌 🥜 Edit 賭 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 3 4447634 76470-66-1 5284584 00447 349.769 🗌 🥜 Edit 👫 Copy 🤤 Delete 13 Loracarbel W72I5ZT78Z 1013 C/16\H /16\CIN /3\O/4\ D08143 G32F6EID2H D04049 404903 1359 C/22\H /25\N/3 \O/7\S 🔲 🥜 Edit 👫 Copy 🥥 Delete 14 Ertapenem 4 132758 153832-46-3 150610 00303 475.516 🗌 🥜 Edit 👫 Copy 🤤 Delete 15 Doripenem 4 66040 148016-81-3 73303 BHV525JOBH D0389 C/15\H 420.50 491571 0/6\S/2 C/12\H /17\N/3 \O/4\S 🔲 🥔 Edit 👫 Copy 🤤 Delete 16 Imipenem 4 4445535 74431-23-5 5282372 01598 710TZ9ZE0A 51799 43708 299.347 C/16\H /26\N/2 \O/5\S 🗌 🥒 Edit 🚰 Copy 🤤 Delete 17 Cilastatin 4 4940183 82009-34-5 01597 141A6AMN38 D07698 3697 358.454 5280454 766 🔲 🥔 Edit 👫 Copy 🤤 Delete 18 Meropenem 4 389924 119478-56-7 441130 00760 FV9J3JU8B1 D02222 43968 127 C/17\H /25\N/3 383.464 🗌 🥒 Edit 👫 Copy 🥥 Delete 19 Cefadroxi 5 43629 66592-87-8 47964 01140 280111G160 D02353 53667 1644 C/16\H /17\N/3 363,389 📄 🥜 Edit 👫 Copy 🥥 Delete 20 Cefazolin 5 30723 25953-19-9 33255 01327 IHS69L0Y4T D02299 474053 1435 C/14\H /14\N/8 454 51 C/16\H /16\N/2 \O/6\S/; 🗌 🥒 Edit 👫 Copy 🤤 Delete 21 Cefalotin 5 5802 153-61-7 6024 00456 R72LW146E6 D07635 124991 617 396.44 5 25541 🔲 🥔 Edit 👫 Copy 🥥 Delete 22 Cefalexin 15686-71-2 2666 00567 5SFF1W6677 D00263 3534 1727 C/16\H /17\N/3 347.39 🗌 🥜 Edit 🚰 Copy 🤤 Delete 23 Cefaclor 6 46260 53994-73-3 51038 00833 3Z6FS3IK0K D00256 8867 C/15\H /14\CIN 367.808 🔲 🖉 Edit 賭 Copy 🥥 Delete 24 Cefamandole 6 401748 34444-01-4 456255 01326 5CKP8C2LLI D02344 3480 1146 462.505 C/18\H /18\N/6 🗌 🥜 Edit 👫 Copy 🥥 Delete 25 Cefoxitin 6 389981 C/16\H /17\N/3 35607-66-0 441199 01331 6OEV9DX57Y D02345 209807 996 427.454 6 8063315 92665-29-7 Copy Colete 26 Ceprozil 9887643 01150 1M698F4H4E D07651 3506 1742 C/18\H 389.427 🗌 🥜 Edit 👫 Copy 🤤 Delete 27 Cefuroxime 6 4514699 55268-75-2 5361202 C/16\H /16\N/4 \O/8\S 01112 O1R9FJ93ED D00262 466 424.386 🔲 🥔 Edit 👫 Copy 🤤 Delete 28 Cefixime 7 4514923 🗌 🥒 Edit 👫 Copy 🤤 Delete 29 Cefdinii 7 529170 🗌 🥔 Edit 👫 Copy 🤤 Delete 30 Cefditoren 7 8046534 ↑___ Check All / Uncheck All With selected: 🥜 Change 🔤 Delete 🔜 Export 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 Let every user access this bookmark Label:

Bookmark this SQL query

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