
ARG(Genes de resistencia a antibióticos)

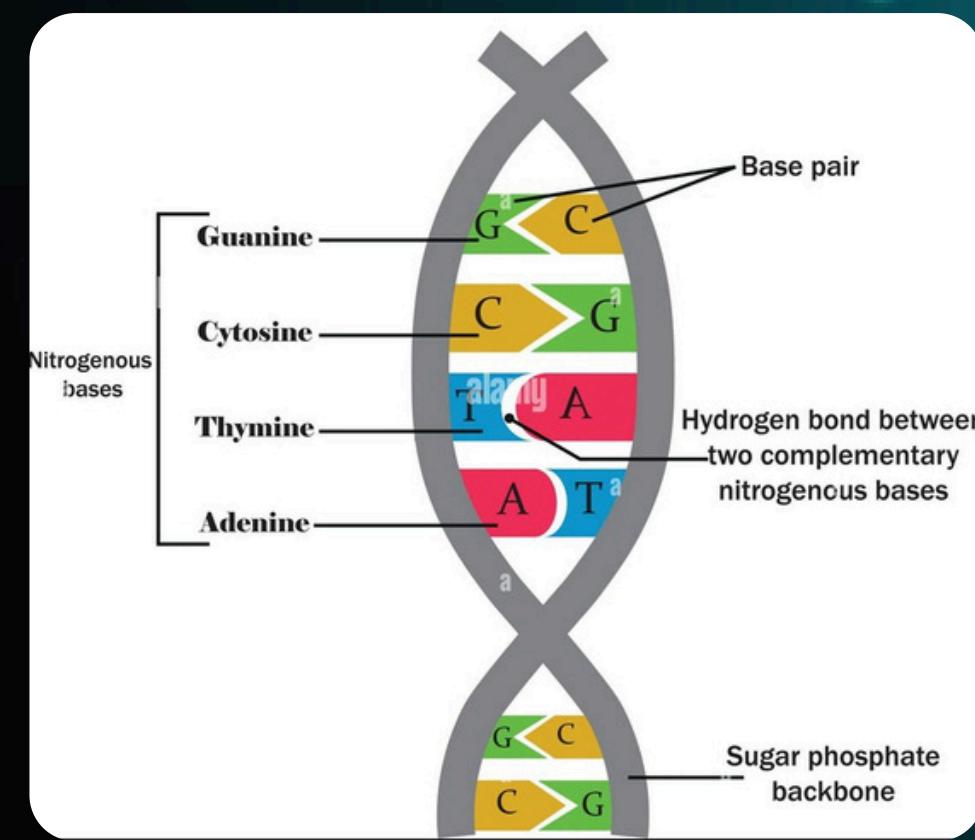
Daniel Navarro Puche, Cintia Rodriguez Aladino, Junjing Wu, Shengkai Zhu

01

INTRODUCCIÓN



¿QUÉ ES UN ARG?



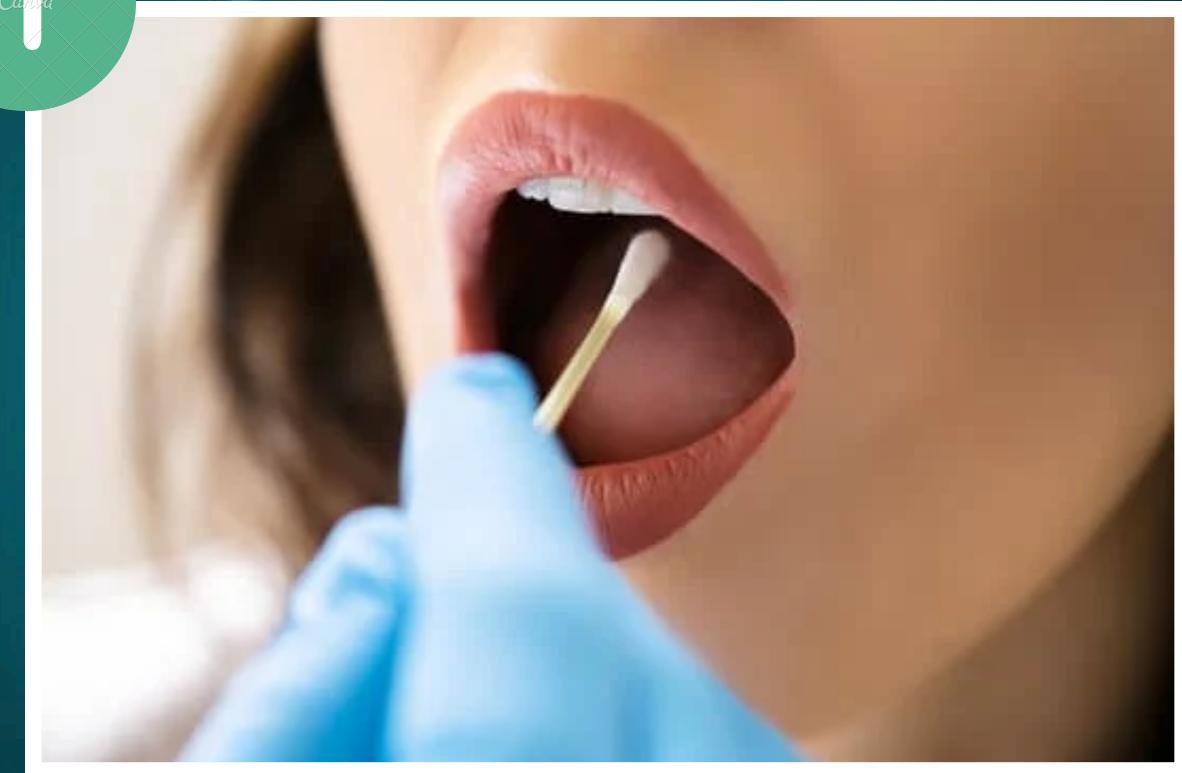
A vertical sequence of DNA nucleotides represented by colored blocks (A, T, C, G) forming a ladder-like pattern. The sequence starts with A (Adenine) and ends with G (Guanine).

Segunda Letra				
	U	C	A	G
U	UUU Phe UUC Phe UUA Leu UUG Leu	UCU Ser UCC Ser UCA Ser UCG Ser	UAU Tyr UAC Tyr UAA STOP UAG STOP	UGU Cys UGC Cys UGA STOP UGG Trp
C	CUU Leu CUC Leu CUA Leu CUG Leu	CCU Pro CCC Pro CCA Pro CCG Pro	CAU His CAC His CAA Gln CAG Gln	CGU Arg CGC Arg CGA Arg CGG Arg
A	AUU Ile AUC Ile AUA Ile AUG Met	ACU Thr ACC Thr ACA Thr ACG Thr	AAU Asn AAC Asn AAA Lys AAG Lys	AGU Ser AGC Ser AGA Arg AGG Arg
G	GUU Val GUC Val GUA Val GUG Val	GCU Ala GCC Ala GCA Ala GCG Ala	GAU Asp GAC Asp GAA Glu GAG Glu	GGU Gly GGC Gly GGA Gly GGG Gly

- El ADN se compone de 4 nucleóticos: Timina, Adenina, Citosina y Guanina.
- Un gen tiene un tamaño medio de 150 nucleótidos.
- Una mutación en un gen es un cambio en esa secuencia de nucleótidos

¿POR QUÉ ES ÚTIL?

1
Canya



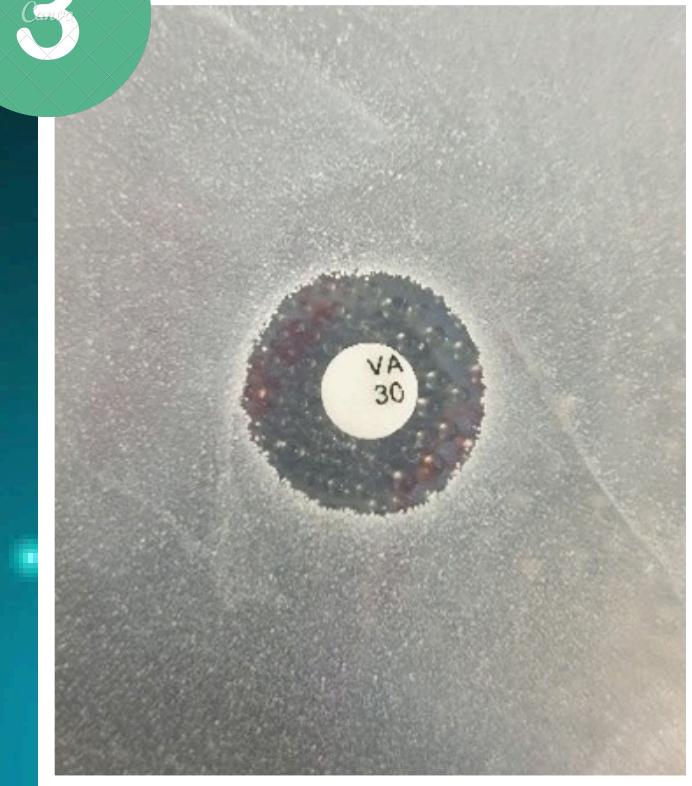
El médico nos receta un antibiótico genérico y posiblemente nos tome una muestra para su análisis en el laboratorio

2



48
HOURS

3



24
HOURS



Se siembra la muestra en varios medios de cultivo para determinar qué bacteria es

Se somete la muestra del paciente a un antibiograma. Aquí se averigua el antibiótico definitivo que será efectivo contra la bacteria

INCOVENIENTES



Pérdida de tiempo



Gasto médico para la SS.



Pérdida de salud para el paciente.



Aumento de resistencias bacterianas.

Evitaremos esto utilizando la técnica de PCR

En general, se tarda mínimo 48h en saber qué microorganismo está causando una infección, a veces hasta 5 o 7 días, dependiendo de la localización y el contexto. Es por eso, que inicialmente se pauta un tratamiento empírico teniendo en cuenta cuál es el origen de la infección, porque en función del origen de la infección hay unos microorganismos muy probables, otros muy poco probables y otros prácticamente imposibles. Luego, también se tienen en cuenta las resistencias locales de cada microorganismo, las personales (hay pacientes ya colonizados con multirresistentes), y en función de eso se decide una cosa u otra.

Una vez que se conocen el microorganismo y su sensibilidad, la elección del antibiótico se hace también en función de la localización de la infección por la farmacocinética del fármaco y su biodisponibilidad según qué tejidos, o si se excreta por orina o se metaboliza en el hígado y se coge el antibiótico de menos espectro que tenga buena CMI, para minimizar resistencias.

Raquel Fernández Tajuelo, Médico intensivista

A Food Poisoning Caused by *Salmonella Enterica* (*S. Enteritidis*) ST11 Carrying Multi-Antimicrobial Resistance Genes in 2019, China

Zhiyi Zhang^{1,2,*}, Baisheng Li^{3,4,*}, Huitao Huang⁵, Yanmei Fang⁵, Wenqiang Yang^{5,✉}

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PMCID: PMC11086652 PMID: [38736437](#)

understand disease transmission routes. Whole-genome sequencing of large numbers of *Salmonella* isolates can be further complemented by the application of mathematical models, combined with machine-learning algorithms that can identify patterns in complex datasets, for better estimates.

02

NUESTROS

DATASET



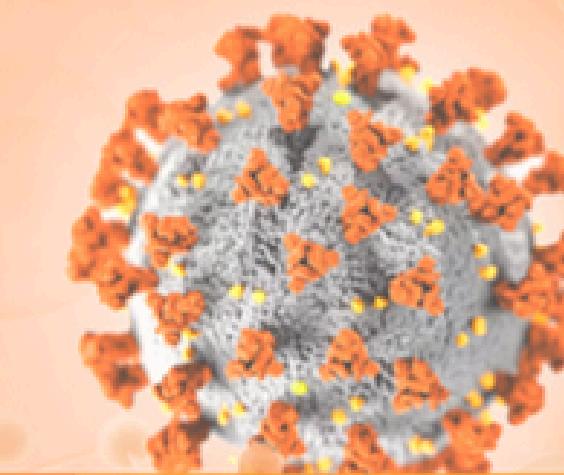
Global Catalogue of Pathogens

A comprehensive pathogenic microbial data sharing center (gcPathogen) serving the field of public health and disease control

Bacteria

Please enter the pathogen name or taxonomy ID

Search

Example : *Bacillus cereus*[Advanced Search](#)

Bacteria

Genomes
1,600,651Taxa
551Strains
1,272,815

Fungi

Genomes
8,791Taxa
442Strains
7,687

Virus

Genomes
119,182Taxa
258Strains
19,089

Parasite

Genomes
782Taxa
180Strains
466

Pathogen names

Taxonomy ID

NO. of Genomes

NO. of ARGs

NO. of VFs

NO. of MGEs

Download

Salmonella enterica	28001	650566	761	201	2664	±ARG ±VF ±MGE ±FAST
Escherichia coli	562	283100	1231	301	3595	±ARG ±VF ±MGE ±FAST
Staphylococcus aureus	1280	94080	209	80	667	±ARG ±VF ±MGE ±FAST
Campylobacter jejuni	197	81460	181	30	84	±ARG ±VF ±MGE ±FAST
Klebsiella pneumoniae	573	75087	1326	169	2002	±ARG ±VF ±MGE ±FAST
Listeria monocytogenes	1639	63011	109	72	140	±ARG ±VF ±MGE ±FAST
Streptococcus pneumoniae	1313	46052	175	100	145	±ARG ±VF ±MGE ±FAST
Campylobacter coli	195	33144	119	18	89	±ARG ±VF ±MGE ±FAST
Pseudomonas aeruginosa	287	31883	885	93	687	±ARG ±VF ±MGE ±FAST
Acinetobacter baumannii	470	29662	1018	90	686	±ARG ±VF ±MGE ±FAST

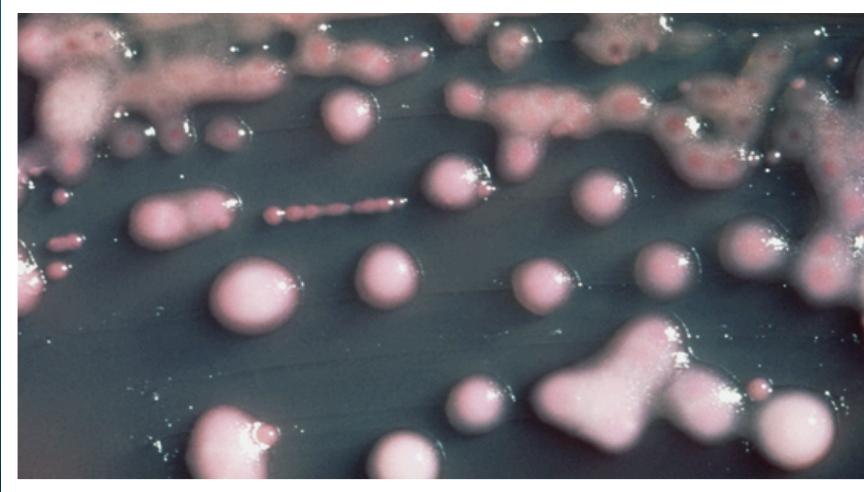
Total 551 < 1 2 3 4 5 6 ... 56 > Go

Enlace:
<https://nmdc.cn/gcpathogen/>

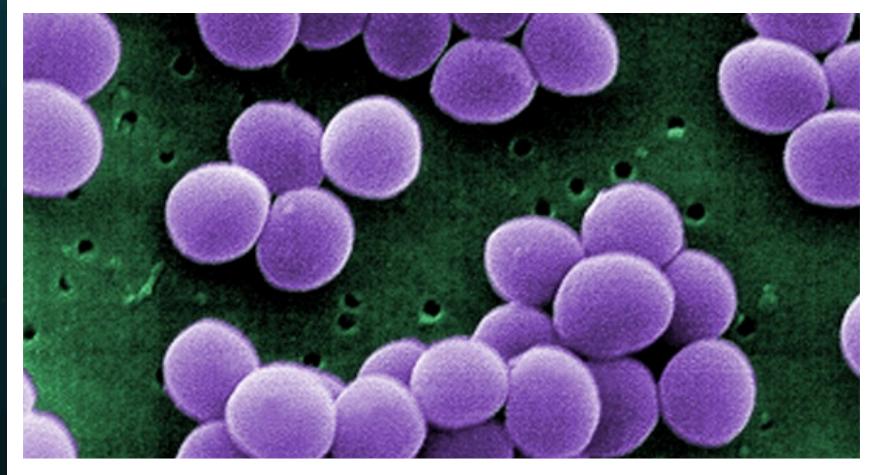
CONTENIDO DEL TSV

1	pathogen_name	taxonid	ARG_name	aro_id	frequency	antibiotic_name	drugclass	associated_PGE_type	associated_PGE_element
2	Salmonella enterica	28901	Tetracycline-resistant ribosomal protection protein	3000002	0.005229			Tetracycline antibiotic	
3	Salmonella enterica	28901	ATP-binding cassette (ABC) antibiotic efflux pump	0010001	0.999999				
4	Salmonella enterica	28901	Major facilitator superfamily (MFS) antibiotic efflux pump	0010002	0.999999				
5	Salmonella enterica	28901	Resistance-nodulation-cell division (RND) antibiotic efflux pump	0010004	0.99855				
6	Salmonella enterica	28901	Determinant of antibiotic resistance	3000000	0.999924				
7	Salmonella enterica	28901	Beta-lactamase	3000001	0.999876				
8	Salmonella enterica	28901	VanH	3000002	0.000002	glycopeptide antibiotic			
9	Salmonella enterica	28901	Class B (metallo-) beta-lactamase	3000004	0.999819				
10	Salmonella enterica	28901	VanH	3000006	0.000011	glycopeptide antibiotic			
11	Salmonella enterica	28901	VanA	3000010	0.000004	glycopeptide antibiotic			
12	Salmonella enterica	28901	VanX	3000011	0.000007	glycopeptide antibiotic			
13	Salmonella enterica	28901	VanB	3000013	0.000002	glycopeptide antibiotic			
14	Salmonella enterica	28901	TDM beta-lactamase	3000014	0.005537	Ampicillin Penam			
15	Salmonella enterica	28901	CTX-M beta-lactamase	3000016	0.020134	Cephalosporin			
16	Salmonella enterica	28901	OXA beta-lactamase	3000017	0.004931	Cefalotin,Cloxacillin,Oxacillin Cephalosporin,Penam			
17	Salmonella enterica	28901	VIM beta-lactamase	3000021	0.000039	Carbapenem,Cephalosporin,Cephemycin,Penam,Penem			
18	Salmonella enterica	28901	ESBL	3000027	0.019387	Fluoroquinolone antibiotic			
19	Salmonella enterica	28901	VLB beta-lactamase	3000043	0.000015	Cephalosporin,Monobactam			
20	Salmonella enterica	28901	PER beta-lactamase	3000056	0.000015	Carbapenem,Cephalosporin,Monobactam,Penam,Penem			
21	Salmonella enterica	28901	NDM beta-lactamase	3000057	0.000085	Carbapenem,Cephalosporin,Cephemycin,Penam			
22	Salmonella enterica	28901	MIR beta-lactamase	3000058	0.025311	Cephalosporin,Monobactam			
23	Salmonella enterica	28901	KPC beta-lactamase	3000059	0.000015	Carbapenem,Cephalosporin,Monobactam,Penam			
24	Salmonella enterica	28901	FOX beta-lactamase	3000067	0.025311	Cephalosporin,Cephemycin			
25	Salmonella enterica	28901	DHA beta-lactamase	3000068	0.000564	Cephalosporin,Cephemycin			
26	Salmonella enterica	28901	CMY beta-lactamase	3000069	0.025311	Cephemycin			
27	Salmonella enterica	28901	VanS	3000071	0.000009	glycopeptide antibiotic			
28	Salmonella enterica	28901	ACT beta-lactamase	3000072	0.025311	Carbapenem,Cephalosporin,Cephemycin,Penam			
29	Salmonella enterica	28901	BarB	3000074	0.999558	Fluoroquinolone antibiotic plasmid,15	InCHI2A,AP001918(IncFIB),IS110,R27(IncHII),H11(IncFI)		
30	Salmonella enterica	28901	Class D beta-lactamase	3000075	0.0004931				

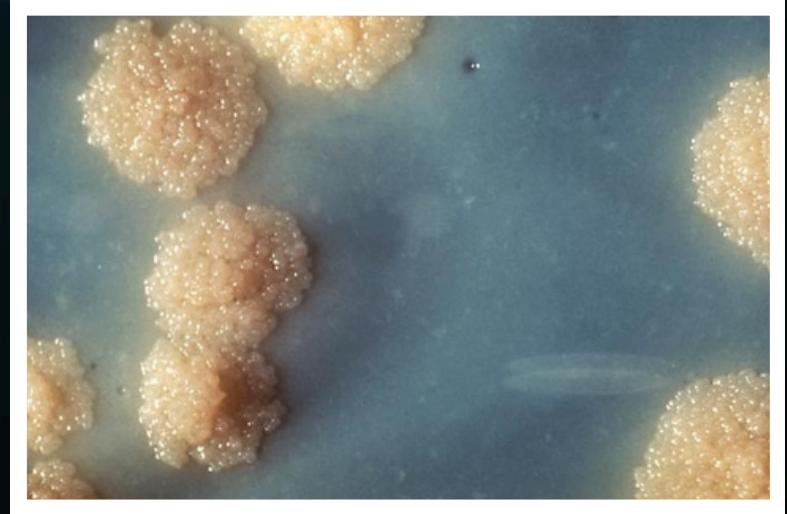
NUESTRAS BACTERIAS



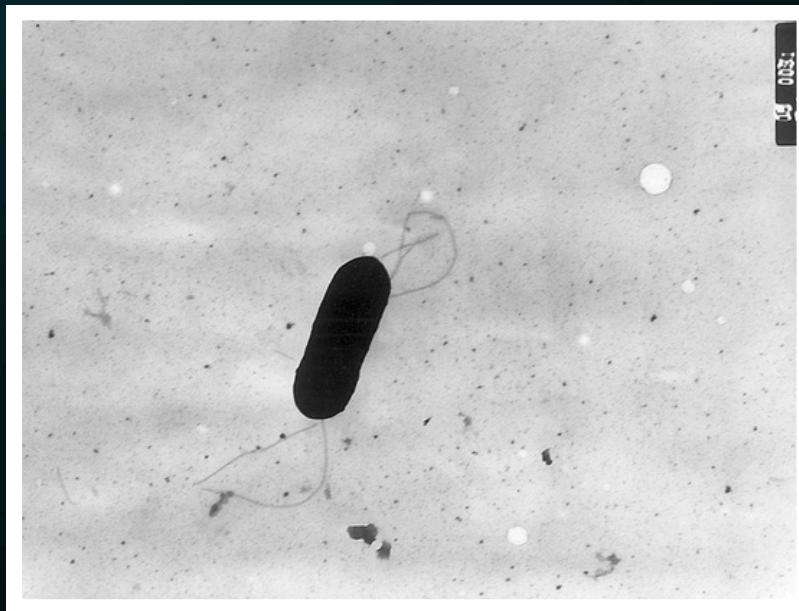
Klebsiella pneumoniae



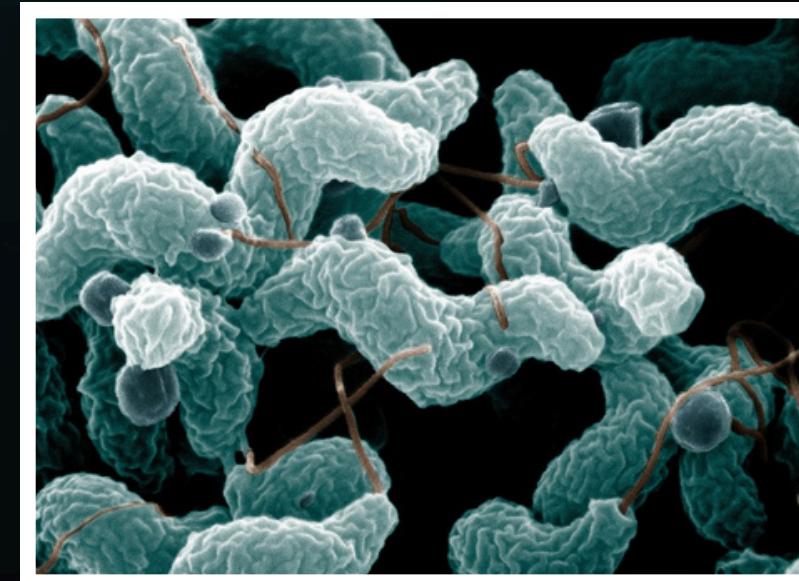
Staphylococcus aureus



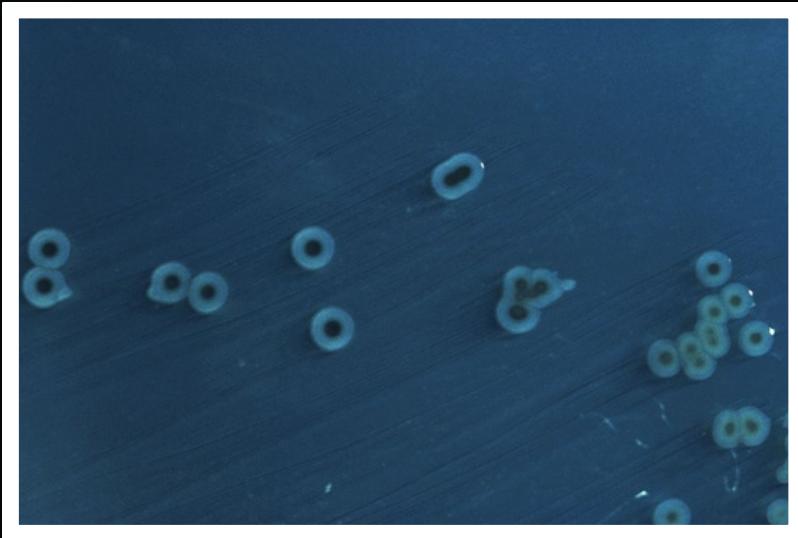
Mycobacterium tuberculosis



Listeria monocytogenes

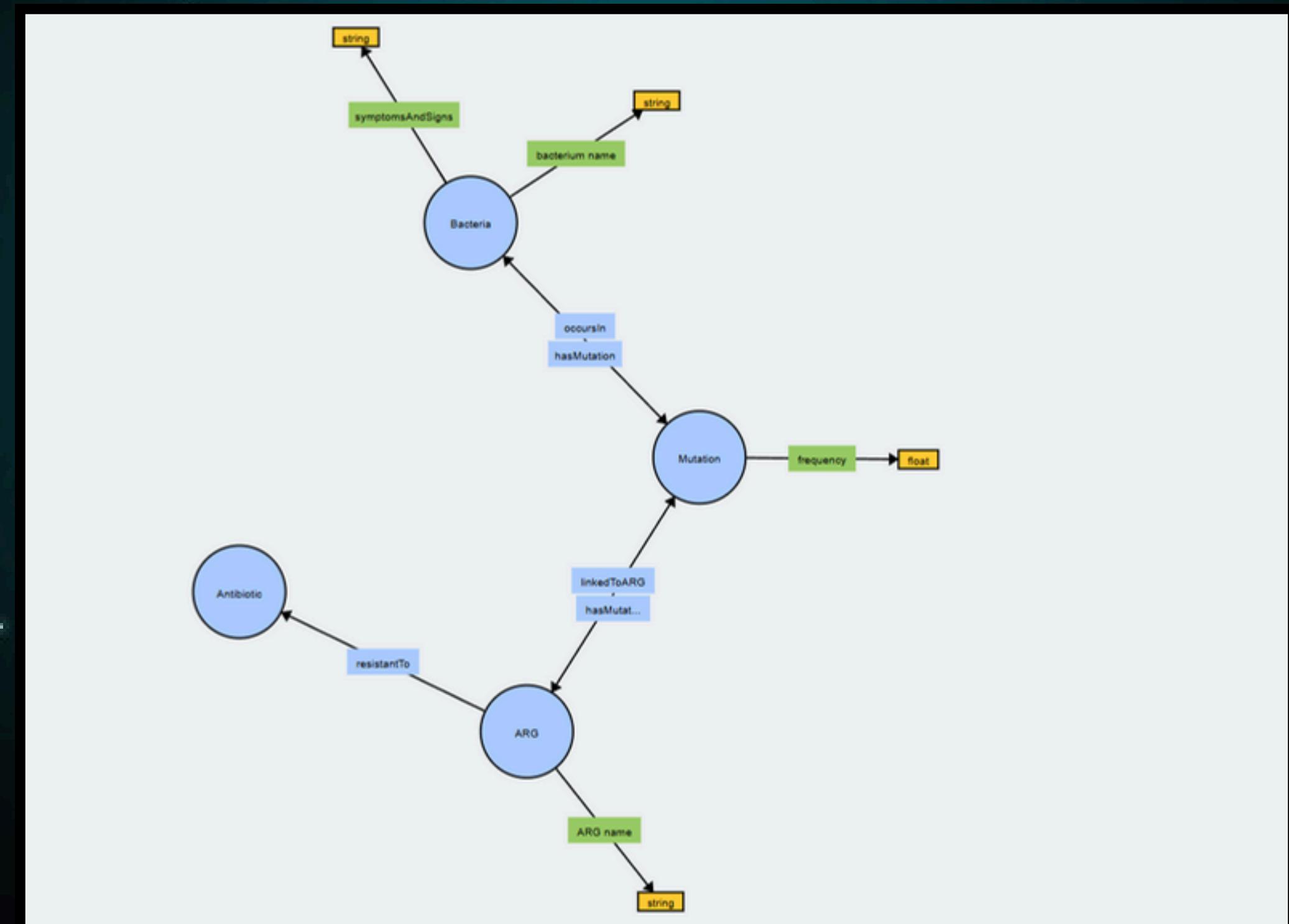


Campylobacter jejuni



Salmonella enterica

ONTOLOGÍA



MAPPING CON OPENREFINE

8397 rows

Show as: rows records Show: 5 10 25 50 100 500 1000 rows « first < previous

All	pathogen_name	has effect	symptoms and signs	taxonid	ARG_name	frequency	antibiotic_name
976.	Mycobacterium tuberculosis	tuberculosis Choose new match	cough,hemoptysis,weight loss,fever,night sweats,chest pain,fatigue,chills	1773	Tet(O)	0.0001380000000000	oxytetracycline Choose new match
977.	Mycobacterium tuberculosis	tuberculosis Choose new match	cough,hemoptysis,weight loss,fever,night sweats,chest pain,fatigue,chills	1773	Tet(O)	0.0001380000000000	tetracycline Choose new match
978.	Mycobacterium tuberculosis	tuberculosis Choose new match	cough,hemoptysis,weight loss,fever,night sweats,chest pain,fatigue,chills	1773	Tet(S)	0.0001380000000000	chlorotetracycline Choose new match
979.	Mycobacterium tuberculosis	tuberculosis Choose new match	cough,hemoptysis,weight loss,fever,night sweats,chest pain,fatigue,chills	1773	Tet(S)	0.0001380000000000	demeclocycline Choose new match
980.	Mycobacterium tuberculosis	tuberculosis Choose new match	cough,hemoptysis,weight loss,fever,night sweats,chest pain,fatigue,chills	1773	Tet(S)	0.0001380000000000	doxycycline Choose new match
981.	Mycobacterium tuberculosis	tuberculosis Choose new match	cough,hemoptysis,weight loss,fever,night sweats,chest pain,fatigue,chills	1773	Tet(S)	0.0001380000000000	minocycline Choose new match
982.	Mycobacterium tuberculosis	tuberculosis Choose new match	cough,hemoptysis,weight loss,fever,night sweats,chest pain,fatigue,chills	1773	Tet(S)	0.0001380000000000	oxytetracycline Choose new match
983.	Mycobacterium tuberculosis	tuberculosis Choose new match	cough,hemoptysis,weight loss,fever,night sweats,chest pain,fatigue,chills	1773	Tet(S)	0.0001380000000000	tetracycline Choose new match
984.	Mycobacterium tuberculosis	tuberculosis Choose new match	cough,hemoptysis,weight loss,fever,night sweats,chest pain,fatigue,chills	1773	Tet(W)	0.0001380000000000	chlorotetracycline Choose new match
985.	Mycobacterium tuberculosis	tuberculosis Choose new match	cough,hemoptysis,weight loss,fever,night sweats,chest pain,fatigue,chills	1773	Tet(W)	0.0001380000000000	demeclocycline Choose new match
986.	Mycobacterium tuberculosis	tuberculosis Choose new match	cough,hemoptysis,weight loss,fever,night sweats,chest pain,fatigue,chills	1773	Tet(W)	0.0001380000000000	doxycycline Choose new match
987.	Mycobacterium tuberculosis	tuberculosis Choose new match	cough,hemoptysis,weight loss,fever,night sweats,chest pain,fatigue,chills	1773	Tet(W)	0.0001380000000000	minocycline Choose new match
988.	Mycobacterium tuberculosis	tuberculosis Choose new match	cough,hemoptysis,weight loss,fever,night sweats,chest pain,fatigue,chills	1773	Tet(W)	0.0001380000000000	oxytetracycline Choose new match
989.	Mycobacterium tuberculosis	tuberculosis Choose new match	cough,hemoptysis,weight loss,fever,night sweats,chest pain,fatigue,chills	1773	Tet(W)	0.0001380000000000	tetracycline Choose new match
990.	Mycobacterium tuberculosis	tuberculosis Choose new match	cough,hemoptysis,weight loss,fever,night sweats,chest pain,fatigue,chills	1773	AcrB	0.9746140000000000	Cephalosporin Choose new match
991.	Mycobacterium tuberculosis	tuberculosis Choose new match	cough,hemoptysis,weight loss,fever,night sweats,chest pain,fatigue,chills	1773	AcrB	0.9746140000000000	Disinfecting agents and antiseptics <small>new</small> Choose new match
992.	Mycobacterium tuberculosis	tuberculosis Choose new match	cough,hemoptysis,weight loss,fever,night sweats,chest pain,fatigue,chills	1773	AcrB	0.9746140000000000	fluoroquinolone Choose new match
993.	Mycobacterium tuberculosis	tuberculosis Choose new match	cough,hemoptysis,weight loss,fever,night sweats,chest pain,fatigue,chills	1773	AcrB	0.9746140000000000	penam Choose new match
994.	Mycobacterium tuberculosis	tuberculosis Choose new match	cough,hemoptysis,weight loss,fever,night sweats,chest pain,fatigue,chills	1773	AcrB	0.9746140000000000	amphenicols Choose new match
995.	Mycobacterium tuberculosis	tuberculosis Choose new match	cough,hemoptysis,weight loss,fever,night sweats,chest pain,fatigue,chills	1773	AcrB	0.9746140000000000	rifamycin Choose new match
996.	Mycobacterium tuberculosis	tuberculosis Choose new match	cough,hemoptysis,weight loss,fever,night sweats,chest pain,fatigue,chills	1773	AcrB	0.9746140000000000	tetracycline antibiotic Choose new match
997.	Mycobacterium tuberculosis	tuberculosis Choose new match	cough,hemoptysis,weight loss,fever,night sweats,chest pain,fatigue,chills	1773	ANT(9)	0.0002780000000000	aminoglycoside antibiotic Choose new match
998.	Mycobacterium tuberculosis	tuberculosis Choose new match	cough,hemoptysis,weight loss,fever,night sweats,chest pain,fatigue,chills	1773	ANT(3')-la	0.0001380000000000	aminoglycoside antibiotic Choose new match
999.	Mycobacterium tuberculosis	tuberculosis Choose new match	cough,hemoptysis,weight loss,fever,night sweats,chest pain,fatigue,chills	1773	RbpA	0.9957230000000000	rifabutin Choose new match
1000.	Mycobacterium tuberculosis	tuberculosis	cough,hemoptysis,weight loss,fever,night sweats,chest pain,fatigue,chills	1773	RbpA	0.9957230000000000	rifampicin Choose new match

RESULTADO DEL MAPPING

```
@prefix ont: <https://Junjingw.github.io/bacteria-ontologia> .
@prefix rdf: <http://www.w3.org/1999/02/22-rdf-syntax-ns#> .
@prefix owl: <http://www.w3.org/2002/07/owl#> .
@prefix rdfs: <http://www.w3.org/2000/01/rdf-schema#> .
@prefix foaf: <http://xmlns.com/foaf/0.1/> .

<https://bacterias#0> a ont:Mutation;
ont:frequency "0.1214800000000000"^^<http://www.w3.org/2001/XMLSchema#double>;
ont:linkedToARG <https://bacterias#/Tetracycline-resistant%20ribosomal%20protection%20protein>;
ont:occursIn <https://bacterias#/Staphylococcus%20aureus> .
<https://bacterias#/Staphylococcus%20aureus> a ont:Bacteria;
ont:taxonId "1280"^^<http://www.w3.org/2001/XMLSchema#int>;
ont:hasMutation <https://bacterias#0>;
foaf:name "Staphylococcus aureus" .
<https://bacterias#/Tetracycline-resistant%20ribosomal%20protection%20protein> a ont:ARG;
ont:hasMutationARG <https://bacterias#0>;
ont:resistantTo <https://bacterias#/Tetracycline%20antibiotic%0D>;
foaf:name "Tetracycline-resistant ribosomal protection protein" .
<https://bacterias#/Tetracycline%20antibiotic%0D> a ont:Antibiotic;
foaf:name """Tetracycline antibiotic
"" .

<https://bacterias#1> ont:linkedToARG <https://bacterias#VanH>;
a ont:Mutation;
ont:frequency "0.00053000000000"^^<http://www.w3.org/2001/XMLSchema#double>;
ont:occursIn <https://bacterias#/Staphylococcus%20aureus> .
<https://bacterias#/Staphylococcus%20aureus> a ont:Bacteria;
ont:taxonId "1280"^^<http://www.w3.org/2001/XMLSchema#int>;
ont:hasMutation <https://bacterias#1>;
foaf:name "Staphylococcus aureus" .
<https://bacterias#VanH> a ont:ARG;
ont:hasMutationARG <https://bacterias#1>;
ont:resistantTo <https://bacterias#/glycoPeptide%20antibiotic%0D>;
foaf:name "VanH" .
<https://bacterias#/glycoPeptide%20antibiotic%0D> a ont:Antibiotic;
foaf:name """glycoPeptide antibiotic
"" .

<https://bacterias#2> a ont:Mutation;
ont:frequency "0.00054400000000"^^<http://www.w3.org/2001/XMLSchema#double>;
ont:linkedToARG <https://bacterias#VanA>;
ont:occursIn <https://bacterias#/Staphylococcus%20aureus> .
<https://bacterias#/Staphylococcus%20aureus> a ont:Bacteria;
ont:taxonId "1280"^^<http://www.w3.org/2001/XMLSchema#int>;
ont:hasMutation <https://bacterias#2>;
foaf:name "Staphylococcus aureus" .
<https://bacterias#VanA> a ont:ARG;
ont:hasMutationARG <https://bacterias#2>;
ont:resistantTo <https://bacterias#/glycoPeptide%20antibiotic%0D>;
foaf:name "VanA" .
```

MAPPING USANDO PYTHON

```
qualifiers_hashmap = dict()
def get_qualifier(name: str) -> str:
    ...

    Get the qualifier of a bacteria with a given name.
    Connects to wikidata search and performs webscraping to get the best
    possible qualifier based on the Levenshtein distance (edit distance) and
    the height of the search result.

    Args:
        name (str): The name of a bacteria.
    Returns:
        str: The qualifier of that bacteria.
    ...

    if name in qualifiers_hashmap:
        return qualifiers_hashmap[name]

    html_content = requests.get(
        'https://www.wikidata.org/w/index.php'
        f'?search={name}',
    ).text
    soup = BeautifulSoup(html_content, 'html.parser')

    search_results = soup.find_all(
        attrs={'class': 'mw-search-result mw-search-result-ns-0'}
    )

    label_index_qualifier_hashmap = dict()
    for i, search_result in enumerate(search_results):
        qualifier = search_result.find(
            attrs={'class': 'wb-itemlink-id'}
        ).contents[0][1:-1]

        label_html = search_result.find(
            attrs={'class': 'wb-itemlink-label'}
        )
        segments = []
        for content in label_html.contents:
            if isinstance(content, NavigableString):
                segment = content
            else:
                segment = content.contents[0]
            segments.append(segment)

        label = ''.join(segments)
        label_index_qualifier_hashmap[(label, i)] = qualifier
```

```
signs_hashmap = dict()
def get_signs(qualifier: str) -> set[str]:
    ...

    Get the signs of a bacteria with a given qualifier. Connects to the sparql
    endpoint of wikidata to query for the signs of the bacteria which are every
    effect, symptom and cause of the bacteria.

    Args:
        qualifier (str): The qualifier of a bacteria.
    Returns:
        set: The signs of that bacteria.
    ...

    if qualifier in signs_hashmap:
        return signs_hashmap[qualifier]

    query_endpoint = 'https://query.wikidata.org/sparql'
    query = '''
    SELECT
        ?effectLabel
        ?dataLabel
    WHERE{
        wd:'''+qualifier+''' wdt:P1542 ?effect .
        OPTIONAL (?effect wdt:P780 ?data)
        SERVICE wikibase:label { bd:serviceParam wikibase:language "en". }
    }
    '''

    params = {'query': query, 'format': 'json'}
    result = json.loads(requests.get(query_endpoint, params=params).text)

    signs = set()
    for entry in result['results']['bindings']:
        signs.add(entry['effectLabel']['value'])
        if 'dataLabel' in entry:
            signs.add(entry['dataLabel']['value'])

    signs_hashmap[qualifier] = signs
    return signs
```

RESULTADO

```
<https://junjingw.github.io/bacteria-ontologia//data/bac3> a ns1:Bacteria ;
    ns1:hasMutation <https://junjingw.github.io/bacteria-ontologia//data/mut296> ,
        <https://junjingw.github.io/bacteria-ontologia//data/mut407> ,
        <https://junjingw.github.io/bacteria-ontologia//data/mut408> ,
        <https://junjingw.github.io/bacteria-ontologia//data/mut409> ,
        <https://junjingw.github.io/bacteria-ontologia//data/mut410> ,
        <https://junjingw.github.io/bacteria-ontologia//data/mut411> ,
        <https://junjingw.github.io/bacteria-ontologia//data/mut412> ;
    ns1:hasSign "chest pain",
        "chills",
        "cough",
        "fatigue",
        "fever",
        "hemoptysis",
        "night sweats",
        "tuberculosis",
        "weight loss" ;
    ns1:taxonId 1773 .
```

03

NUESTRAS

QUERIES



QUERY 1:

ARG más probable y menos probable de cada bacteria.



QUERY 1

```
SELECT ?bacteria_name ?arg_max_name ?freq_max ?arg_min_name ?freq_min WHERE {
  {
    SELECT ?bacteria (MAX(?frequency) AS ?freq_max) (MIN(?frequency) AS ?freq_min)
    WHERE {
      ?mutation ont:occursIn ?bacteria ;
                 ont:linkedToARG ?arg ;
                 ont:frequency ?frequency.
    }
    GROUP BY ?bacteria
  }
  {
    SELECT ?bacteria ?freq_max (SAMPLE(?arg_max_name) AS ?arg_max_name)
    WHERE {
      ?mutation ont:occursIn ?bacteria ;
                 ont:linkedToARG ?arg_max ;
                 ont:frequency ?freq_max.
      ?arg_max foaf:name ?arg_max_name.
    }
    GROUP BY ?bacteria ?freq_max
  }
  {
    SELECT ?bacteria ?freq_min (SAMPLE(?arg_min_name) AS ?arg_min_name)
    WHERE {
      ?mutation ont:occursIn ?bacteria ;
                 ont:linkedToARG ?arg_min ;
                 ont:frequency ?freq_min.
      ?arg_min foaf:name ?arg_min_name.
    }
    GROUP BY ?bacteria ?freq_min
  }
  ?bacteria foaf:name ?bacteria_name.
}
GROUP BY ?bacteria_name ?arg_max_name ?freq_max ?arg_min_name ?freq_min
```

RESULTADOS

	bacteria_name	arg_max_name	freq_max	arg_min_name	freq_min
1	"Staphylococcus aureus"	"MarR"	"0.9999590000000000""xsd:double	"ADC-103"	"0.0000140000000000""xsd:double
2	"Listeria monocytogenes"	"MarR"	"0.9998460000000000""xsd:double	"Cfr(D)"	"0.0000190000000000""xsd:double
3	"Mycobacterium tuberculosis"	"Trimethoprim resistant dihydrofolate reductase dfr"	"0.9993100000000000""xsd:double	"OXA-923"	"0.0001380000000000""xsd:double
4	"Campylobacter jejuni"	"AcrF"	"0.9999820000000000""xsd:double	"QacG"	"0.0000180000000000""xsd:double
5	"Salmonella enterica"	"MarR"	"0.9998720000000000""xsd:double	"MCR-5.3"	"0.0000020000000000""xsd:double
6	"Klebsiella pneumoniae"	"AcrB"	"0.9930100000000000""xsd:double	"KPC-95"	"0.0000210000000000""xsd:double

QUERY 2:

Dada una lista de ARG's determinar
que bacteria podria ser



QUERY 2

```
1 PREFIX ont: <https://Junjingw.github.io/bacteria-ontologia#>
2 PREFIX rdfs: <http://www.w3.org/2000/01/rdf-schema#>
3 PREFIX foaf: <http://xmlns.com/foaf/0.1/>
4
5 SELECT DISTINCT ?bacteria ?bacteriaName ?argName
6 WHERE {
7   ?mutation ont:linkedToARG ?arg ;
8     ont:occursIn ?bacteria .
9   ?bacteria foaf:name ?bacteriaName .
10  ?arg foaf:name ?argName .
11
12  VALUES ?argName { "VanR" "OpmB" }
13 }
```



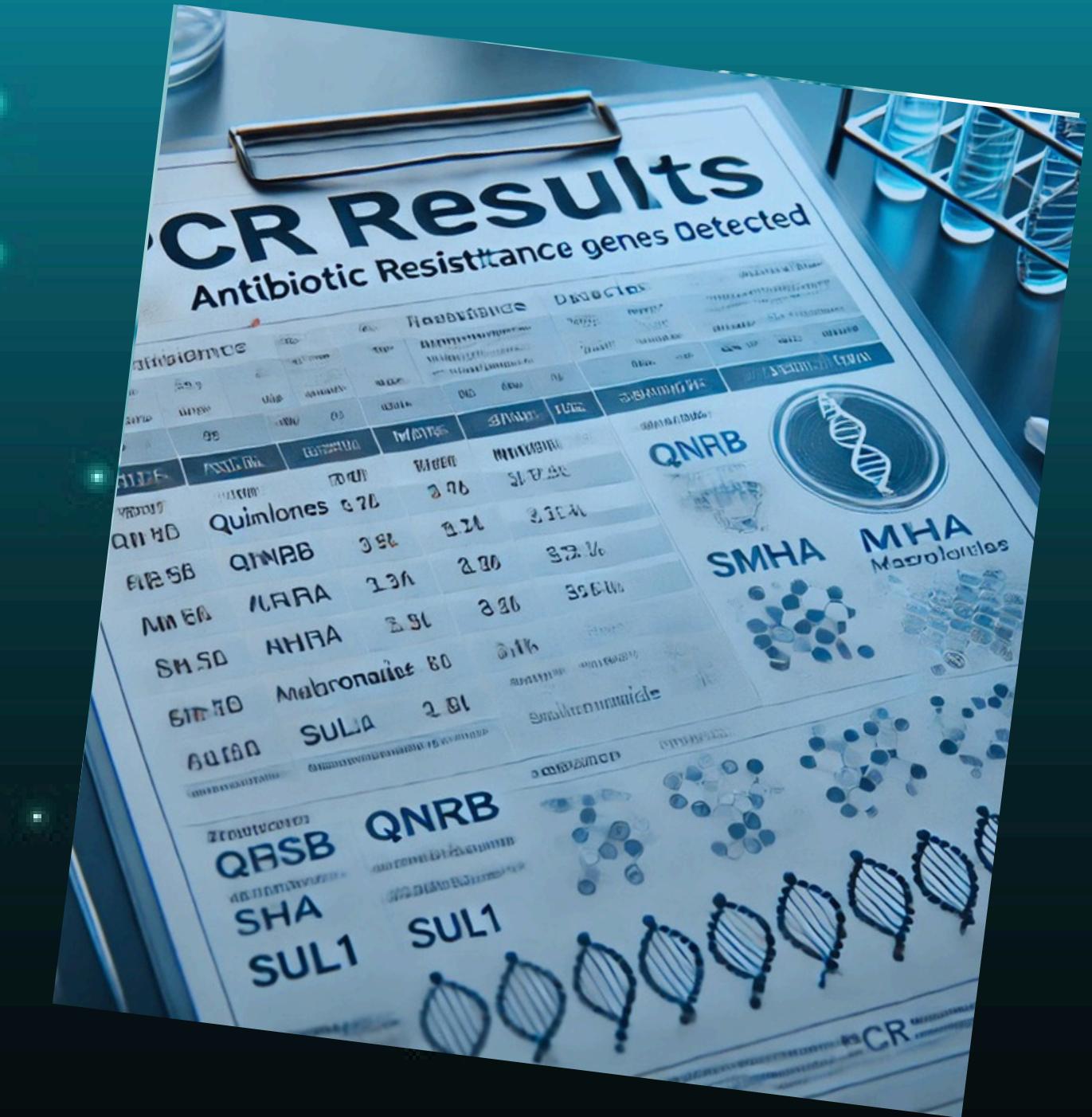
keyboard shortcuts

RESULTADOS

bacteria	bacteriaName	argName
1 https://bacterias#/Staphylococcus%20aureus	"Staphylococcus aureus"	"VanR"
2 https://bacterias#/Listeria%20monocytogenes	"Listeria monocytogenes"	"VanR"
3 https://bacterias#/Mycobacterium%20tuberculosis	"Mycobacterium tuberculosis"	"VanR"
4 https://bacterias#/Campylobacter%20jejuni	"Campylobacter jejuni"	"VanR"
5 https://bacterias#/Salmonella%20enterica	"Salmonella enterica"	"VanR"
6 https://bacterias#/Klebsiella%20pneumoniae	"Klebsiella pneumoniae"	"VanR"
7 https://bacterias#/Klebsiella%20pneumoniae	"Klebsiella pneumoniae"	"OpmB"

QUERY 3:

Simplemente con la muestra se hace una PCR que nos da los ARG, que metemos para saber qué antibióticos descartar por ellos y evitar su consumo.



ARG Detectados :

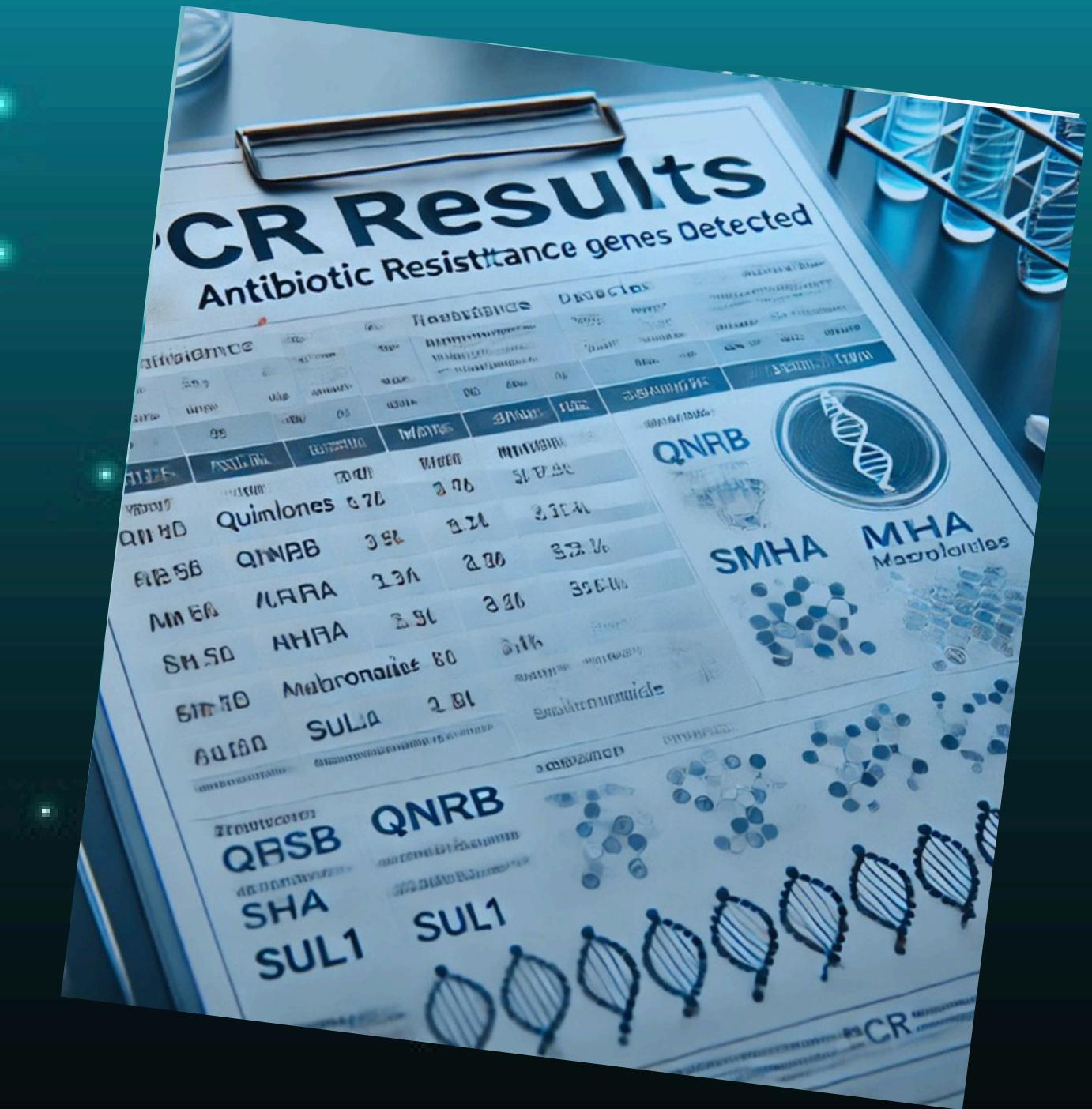
- MdtB
- TolC
- YajC

```
1 PREFIX ont: <https://Junjingw.github.io/bacteria-ontologia#>
2 PREFIX foaf: <http://xmlns.com/foaf/0.1/>
3
4 SELECT ?argName ?antibioticName
5 WHERE {
6     ?arg a ont:ARG ;
7         foaf:name ?argName ;
8         ont:resistantTo ?antibiotic.
9     ?antibiotic foaf:name ?antibioticName.
10
11    VALUES ?argName { "MdtB" "TolC" "YajC" }
12 }
```

	argName	antibiotic_name
1	"MdtB"	"Aminocoumarin antibiotic"
2	"TolC"	"CarbaPenem"
3	"TolC"	"Cephalosporin"
4	"TolC"	"Penam"
5	"TolC"	"Cepharmycin"
6	"TolC"	"Phenicol antibiotic"
7	"TolC"	"Disinfecting agents and antiseptics"
8	"TolC"	"Fluoroquinolone antibiotic"
9	"TolC"	"Rifamycin antibiotic"
10	"TolC"	"Tetracycline antibiotic"
11	"TolC"	"Aminocoumarin antibiotic"
12	"TolC"	"Aminoglycoside antibiotic"
13	"TolC"	"Macrolide antibiotic"
14	"TolC"	"Penem"
15	"TolC"	"Peptide antibiotic"
16	"YajC"	"Rifampin"
17	"YajC"	"Linezolid"
18	"YajC"	"Vancomycin"

QUERY 4:

Dado una lista de medicamentos, un expediente del paciente y los resultados de la PCR , ir descartando medicamentos



EXPEDIENTE MÉDICO

Expediente Médico del Paciente

- **Nombre:** Juan Pérez
- **Edad:** 35 años
- **Sexo:** Masculino
- **Peso:** 75 kg
- **Historial Médico:**
 - **Alergias:** Sulfonamidas (sulfas).
 - **Condiciones Crónicas:** Insuficiencia renal leve (función renal monitorizada con una TFG de 50 mL/min).
 - **Cirugías previas:** Ninguna relevante.
 - **Medicamentos actuales:** No toma medicamentos regularmente.
 - **Antecedentes Infecciosos:** Episodio previo de gastroenteritis tratado exitosamente con Ceftriaxona.
- **Síntomas Actuales:**
 - Fiebre persistente de 38.5 °C.
 - Dolor abdominal en cuadrante inferior derecho.
 - Diarrea acuosa (4-5 episodios diarios).
 - Debilidad general y deshidratación leve.
- **Pruebas Realizadas:**
 - **PCR:** Identificación de genes de resistencia a antibióticos (ARG).

argName	antibioticName
1 "QnrB10"	"Ciprofloxacin"
2 "MphA"	"Azithromycin"
3 "MphA"	"Clarithromycin"
4 "MphA"	"Dirithromycin"
5 "MphA"	"Erythromycin"
6 "MphA"	"Oleandomycin"
7 "MphA"	"Roxithromycin"
8 "MphA"	"Telithromycin"
9 "Sul1"	"Mafenide"
10 "Sul1"	"Sulfacetamide"
11 "Sul1"	"Sulfadiazine"
12 "Sul1"	"Sulfadimidine"
13 "Sul1"	"Sulfadoxine"
14 "Sul1"	"Sulfamethizole"
15 "Sul1"	"Sulfamethoxazole"
16 "Sul1"	"Sulfasalazine"
17 "Sul1"	"Sulfoxazole"
18 "SHV-12"	"Cefalotin"
19 "SHV-12"	"Ceftazidime"
20 "SHV-12"	"Ceftriaxone"

```

1 PREFIX ont: <https://Junjingw.github.io/bacteria-ontologia#>
2 PREFIX rdfs: <http://www.w3.org/2000/01/rdf-schema#>
3 PREFIX foaf: <http://xmlns.com/foaf/0.1/>
4
5 SELECT DISTINCT ?argName ?antibioticName
6 WHERE {
7   ?bacteria a ont:Bacteria ;
8     foaf:name "Salmonella enterica" ;
9     ont:hasMutation ?mutation .
10
11 ?mutation ont:linkedToARG ?arg .
12 ?arg foaf:name ?argName ;
13   ont:resistantTo ?antibiotic .
14
15 VALUES ?argName { "QnrB10" "MphA" "Sul1" "SHV-12" }
16
17 ?antibiotic foaf:name ?antibioticName .
18 }
```

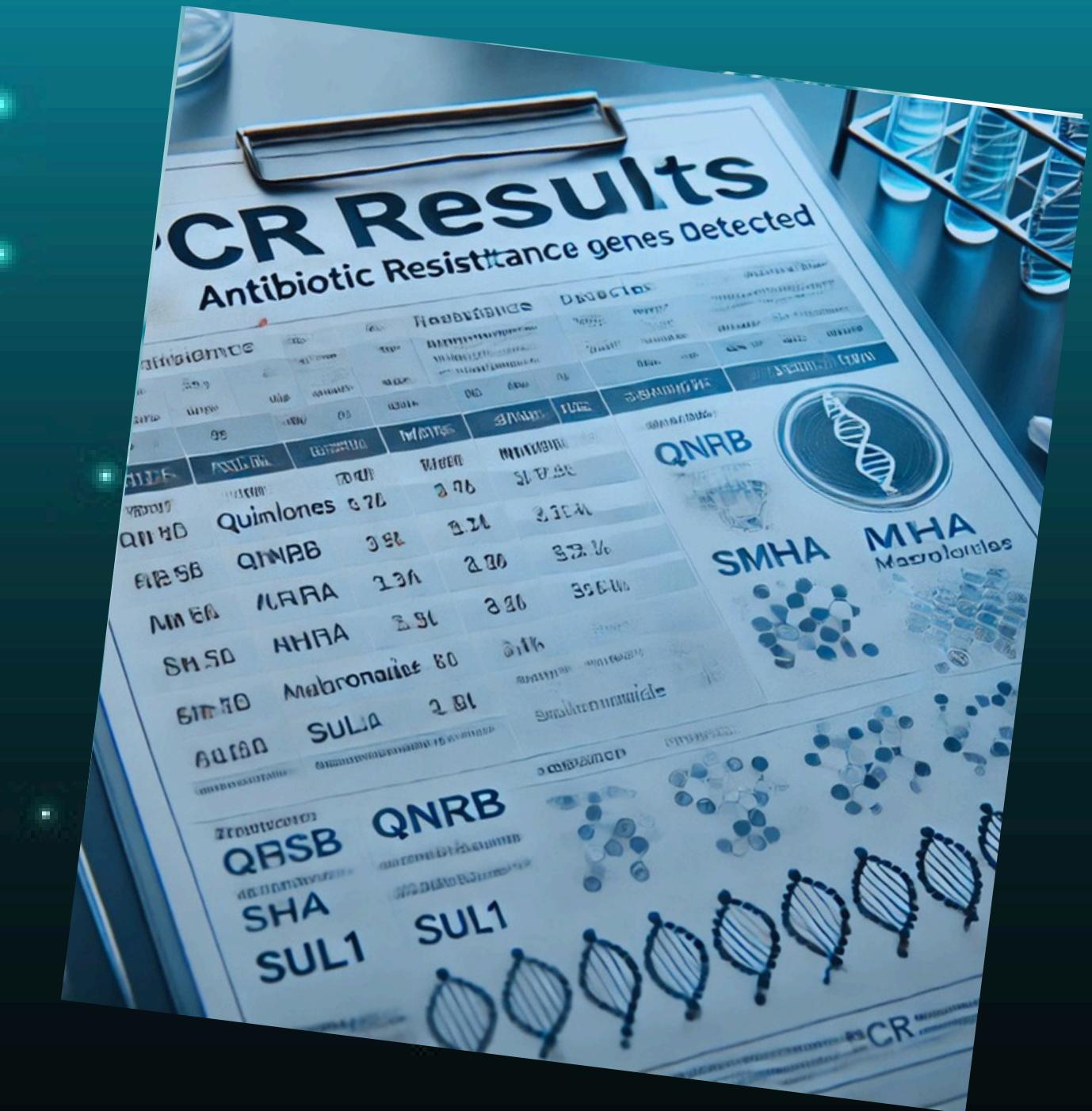
ARG Detectados :

- QnrB10
- MphA
- Sul1
- SHV-12

Medicamento en Español	Medicamento en Inglés	Comentario
[REDACTED]	[REDACTED]	[REDACTED]
[REDACTED]	[REDACTED]	infecciones graves. Evitar en niños y embarazadas.
[REDACTED]	[REDACTED]	en infecciones respiratorias y gastrointestinales.
[REDACTED]	[REDACTED]	para infecciones graves y sistémicas.
Amoxicilina/Ácido clavulánico	Amoxicillin/Clavulanic acid	Muy usado en infecciones comunes, como respiratorias y de piel.
[REDACTED]	[REDACTED]	urinarias y gastrointestinales; evitar en alérgicos a sulfas.

QUERY 5:

Detectar la bacteria a partir de los
sintomas y encontrar el antibiotico
más probable de funcionar.



```
PREFIX foaf: <http://xmlns.com/foaf/0.1/>
PREFIX ont:<https://junjingw.github.io/bacteria-ontologia//ontology#>

SELECT
    ?name
    ?sign
WHERE{
    ?bacteria a ont:Bacteria ;
        ont:hasSign 'fever', 'abortion' .
    ?bacteria foaf:name ?name .
    ?bacteria ont:hasSign ?sign
}
LIMIT 100
```

1	"Listeria monocytogenes"	"abortion"
2	"Listeria monocytogenes"	"anisocoria"
3	"Listeria monocytogenes"	"arachnoiditis"
4	"Listeria monocytogenes"	"blood in stool"
5	"Listeria monocytogenes"	"conjunctivitis"
6	"Listeria monocytogenes"	"diarrhea"
7	"Listeria monocytogenes"	"encephalitis"
8	"Listeria monocytogenes"	"fever"
9	"Listeria monocytogenes"	"hepatomegaly"
10	"Listeria monocytogenes"	"hysteria"
11	"Listeria monocytogenes"	"lymphadenopathy"
12	"Listeria monocytogenes"	"meningitis"
13	"Listeria monocytogenes"	"meningoencephalitis"
14	"Listeria monocytogenes"	"nausea"
15	"Listeria monocytogenes"	"poisoning"
16	"Listeria monocytogenes"	"ptosis"
17	"Listeria monocytogenes"	"sepsis"
18	"Listeria monocytogenes"	"splenomegaly"
19	"Listeria monocytogenes"	"strabismus"
20	"Listeria monocytogenes"	"tonsillitis"
21	"Listeria monocytogenes"	"vomiting"

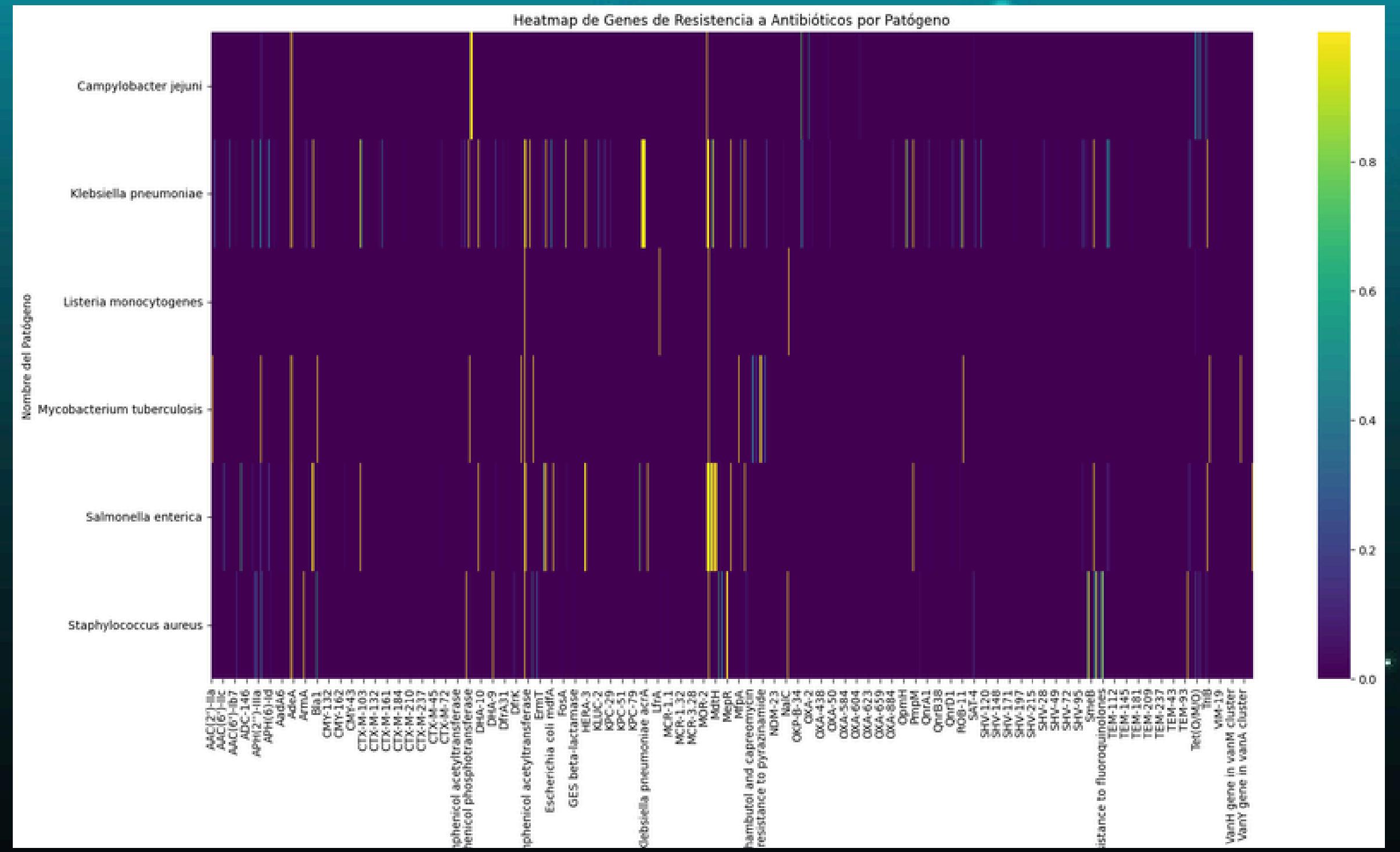
```

PREFIX foaf: <http://xmlns.com/foaf/0.1/>
PREFIX ont:<https://junjingw.github.io/bacteria-ontologia//ontology#>

SELECT
    ?name
    ?arg_name
    ?freq
    ?ant_name
WHERE{
    ?bacteria a ont:Bacteria ;
        ont:hasSign 'fever', 'abortion' .
    ?bacteria foaf:name ?name .
    ?bacteria ont:hasMutation ?mut .
    ?mut ont:linkedToARG ?arg .
    ?arg foaf:name ?arg_name .
    ?mut ont:frequency ?freq .
    ?arg ont:resistantTo ?ant .
    ?ant foaf:name ?ant_name
}
ORDER BY ASC(?freq)
LIMIT 100

```

1	'Listeria monocytogenes'	'MjA'	'1.9e-05'{"label": "float"}	'Fluoroquinolone antibiotic'
2	'Listeria monocytogenes'	'TeoC'	'1.9e-05'{"label": "float"}	'Tetracycline'
3	'Listeria monocytogenes'	'ANT(3')-R'	'1.9e-05'{"label": "float"}	'Aminoglycoside antibiotic'
4	'Listeria monocytogenes'	'MjA'	'1.9e-05'{"label": "float"}	'Aztreomycin'
5	'Listeria monocytogenes'	'MjA'	'1.9e-05'{"label": "float"}	'Telithromycin'
6	'Listeria monocytogenes'	'MjA'	'1.9e-05'{"label": "float"}	'Erythromycin'
7	'Listeria monocytogenes'	'MjA'	'1.9e-05'{"label": "float"}	'Diamidomycin'
8	'Listeria monocytogenes'	'MjA'	'1.9e-05'{"label": "float"}	'Clarithromycin'
9	'Listeria monocytogenes'	'MjA'	'1.9e-05'{"label": "float"}	'Dentromycin'
10	'Listeria monocytogenes'	'MjA'	'1.9e-05'{"label": "float"}	'Rouximycin'
11	'Listeria monocytogenes'	'Sul1'	'1.9e-05'{"label": "float"}	'Sulfamethoxazole'
12	'Listeria monocytogenes'	'Sul1'	'1.9e-05'{"label": "float"}	'Mefenamic acid'



EXPLOTACIÓN DE DATOS

```
from rdflib.plugins.sparql import prepareQuery
import pandas as pd

ont = Namespace("https://junjingw.github.io/bacteria-ontologia//ontology#")

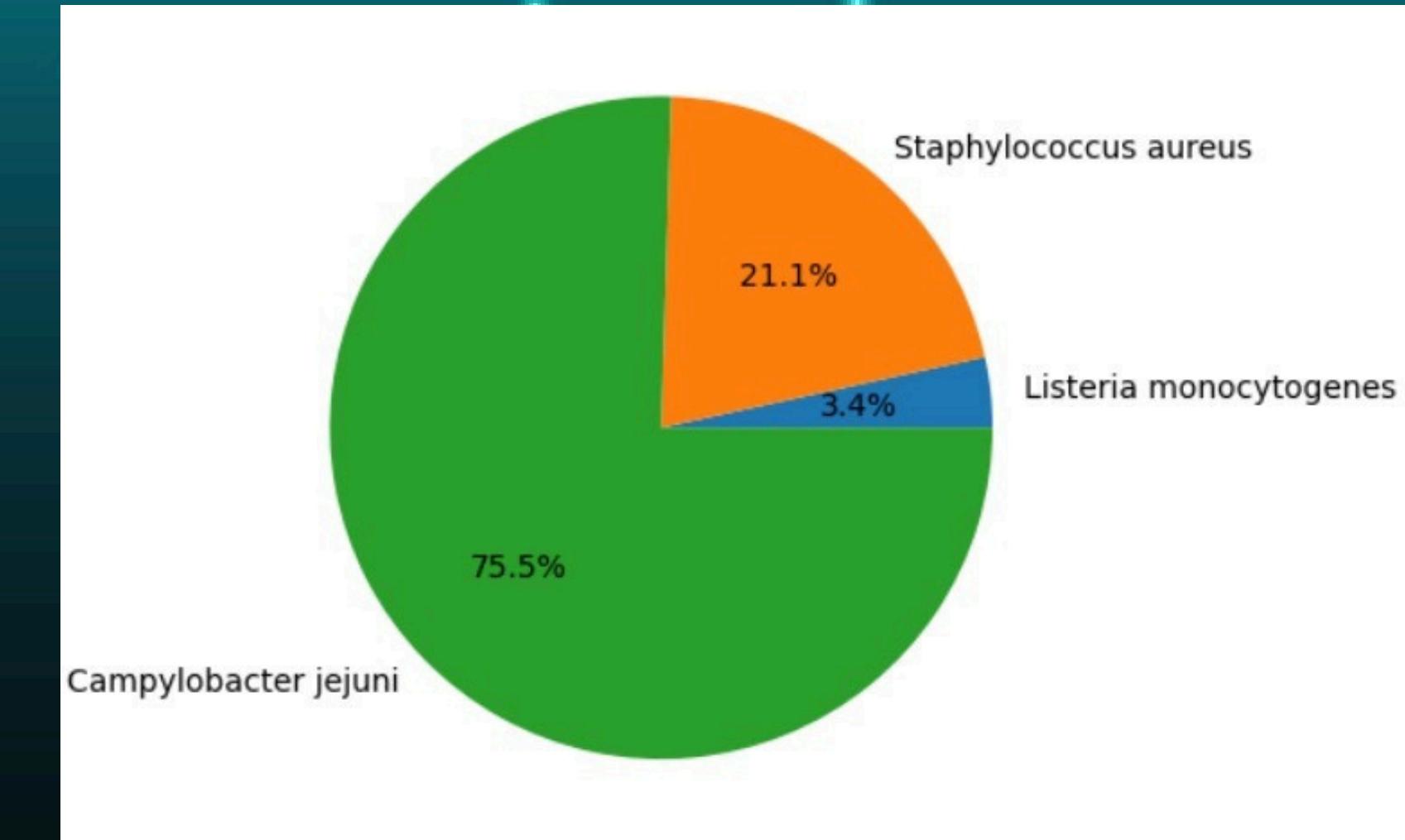
q1 = prepareQuery('''
PREFIX foaf: <http://xmlns.com/foaf/0.1/>

SELECT
  ?bacName
  ?freq
WHERE{
  ?arg foaf:name 'Tet(0)' .
  ?mut ont:linkedToARG ?arg .
  ?mut ont:frequency ?freq .
  ?bac ont:hasMutation ?mut .
  ?bac foaf:name ?bacName
}
ORDER BY ASC(?freq)
LIMIT 100
''',
  initNs = { "ont": ont}
)

data = {}
for r in g.query(q1):
  data[r['bacName'].value] = r['freq'].value

# Filter out small values
threshold = 0.01
filtered_data = {k: v for k, v in data.items() if v >= threshold}

# Plot the pie chart with percentages
pd.Series(filtered_data).plot.pie(autopct='%1.1f%%');
```



```

from rdflib.plugins.sparql import prepareQuery
import pandas as pd

ont = Namespace("https://junjingw.github.io/bacteria-ontologia/ontology#")

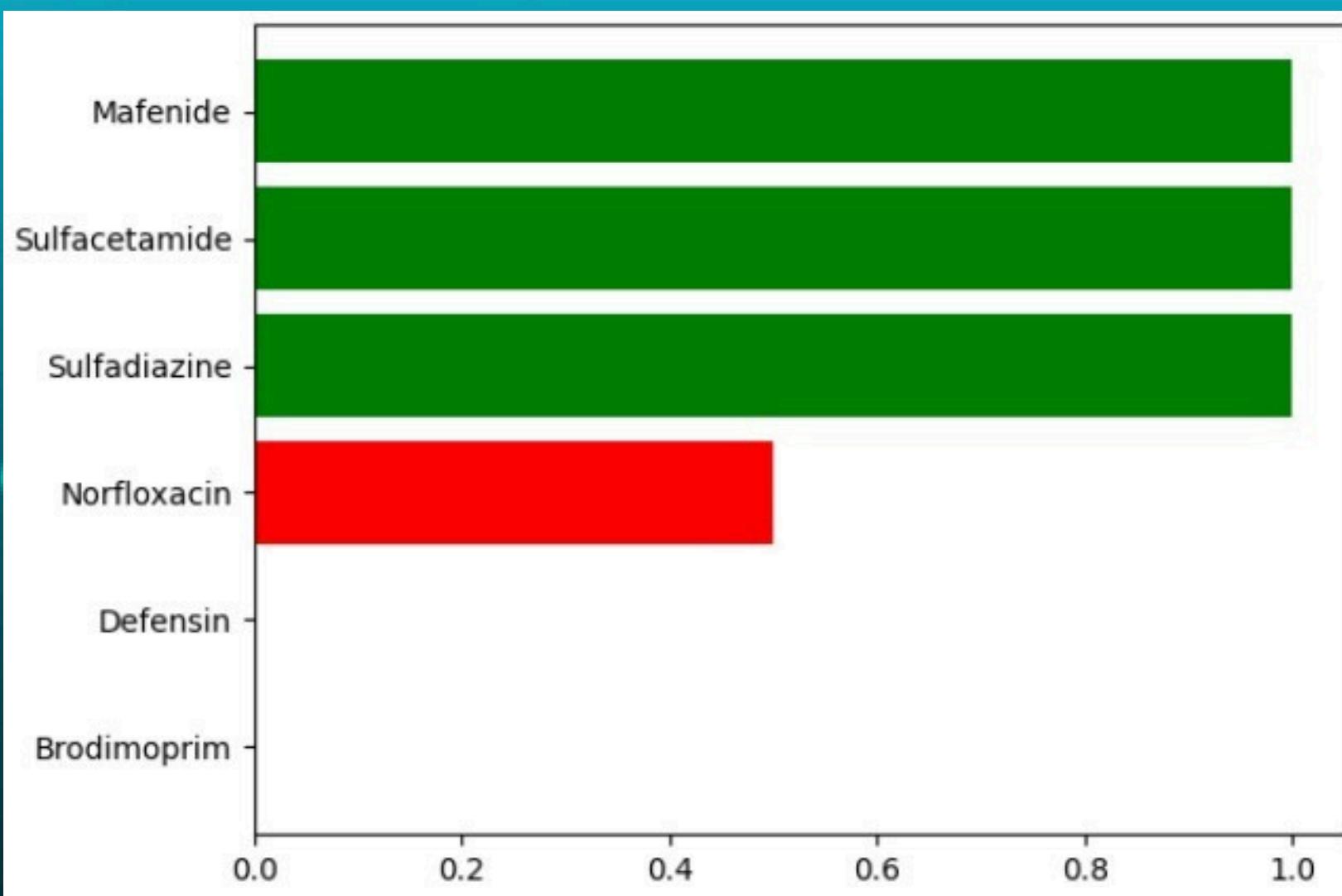
q1 = prepareQuery('''
PREFIX foaf: <http://xmlns.com/foaf/0.1/>
PREFIX ont:<https://junjingw.github.io/bacteria-ontologia/ontology#>

SELECT
    DISTINCT ?ant_name
    (1 - ?avg_freq AS ?probability_to_work)
WHERE{
    SELECT
        ?ant_name
        (AVG(?freq) AS ?avg_freq)
    WHERE{
        ?bacteria a ont:Bacteria ;
        ont:hasSign 'fever', 'abortion' .
        ?bacteria foaf:name ?name .
        ?bacteria ont:hasMutation ?mut .
        ?mut ont:linkedToARG ?arg .
        ?arg foaf:name ?arg_name .
        ?mut ont:frequency ?freq .
        ?arg ont:resistantTo ?ant .
        ?ant foaf:name ?ant_name
    }
    GROUP BY ?ant_name
}
ORDER BY DESC(?probability_to_work)
'''

initNs = { "ont": ont
}

antibiotic_data = {}
for r in g.query(q1):
    antibiotic_data[r['ant_name'].value] = r['probability_to_work'].value
    # data[r['bacName'].value] = r['freq'].value
antibiotic_series = pd.Series(antibiotic_data)
best_and_worst_antibiotics = pd.concat([antibiotic_series.head(3), antibiotic_series.tail(5)[3:]])

```



```

import matplotlib.pyplot as plt

# Define the threshold
threshold = 0.8

# Create a color list based on the threshold
colors = ['green' if value > threshold else 'red' for value in best_and_worst_antibiotics]

# Plot the horizontal bar chart
plt.barrh(best_and_worst_antibiotics.index[::-1], best_and_worst_antibiotics.values[::-1], color=colors[::-1])

# Add labels and title
ax.set_xlabel('Probability to Work')
ax.set_ylabel('Antibiotic')
ax.set_title('Best and Worst Antibiotics')

# Show the plot
plt.show()

```

FIN