Da genômica à pangenômica: predição racional de fármacos e vacinas contra bactérias patogênicas

Siomar de Castro Soares

Origem

Uberaba
289 mil habitantes

Graduação

2002 2004 2006 2008 2010 2012 2014 2016 2018

2003 2005 2007 2009 2011 2013 2015 2017 2019

Graduação em Biomedicina

Uniube

Graduação

2002 2004 2006 2008 2010 2012 2014 2016 2018

2003 2005 2007 2009 2011 2013 2015 2017 2019

Aperfeiçoamento

Aperfeiçoamento em Bioinformática

BIOINFORMÁTICA
UFMG

Pós-Graduação
Genética
UFMG

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Aperfeiçoamento em Bioinformática

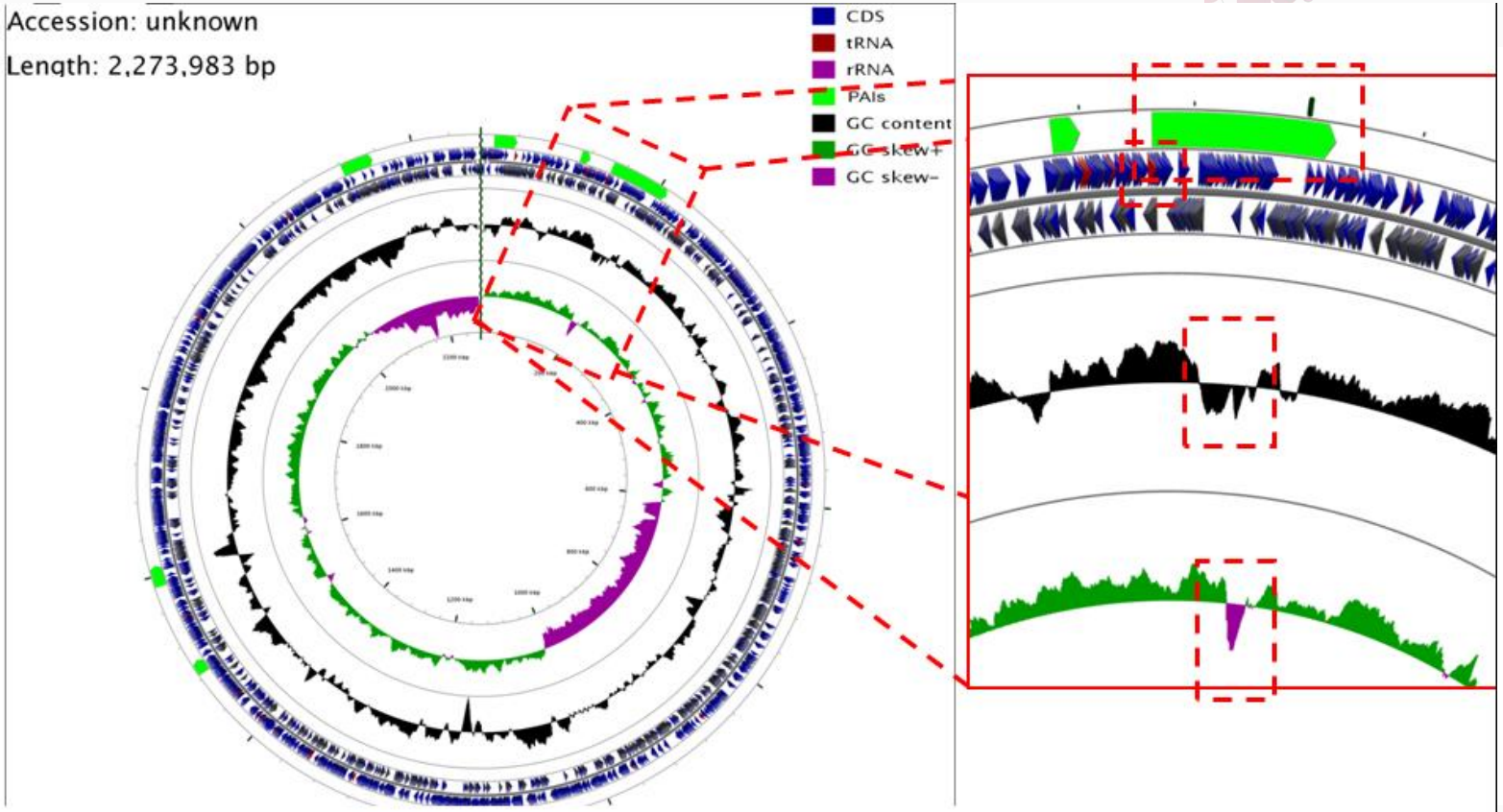

Figure generated using artemis and CGView

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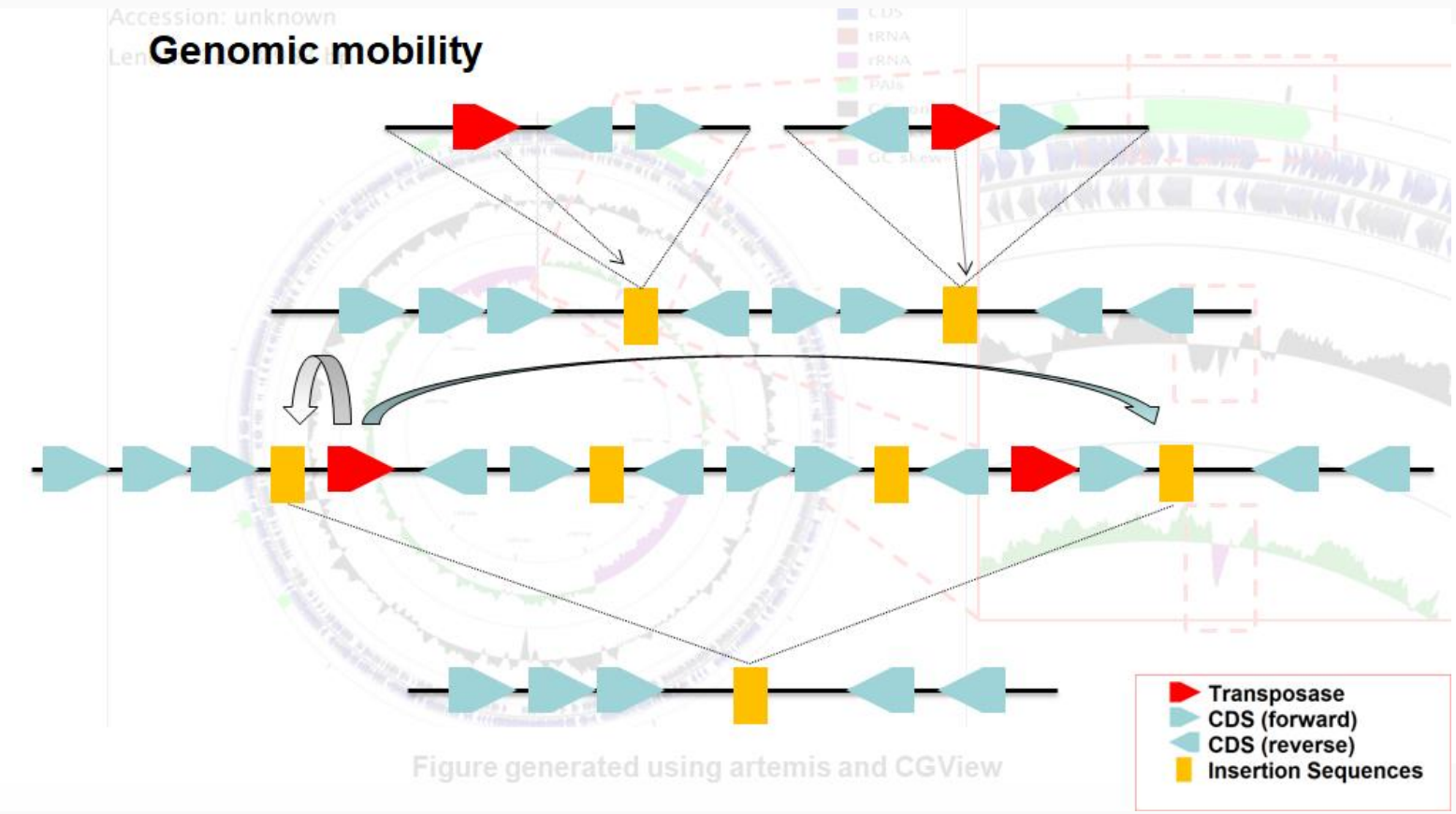
Aperfeiçoamento em Bioinformática



Fatores de virulência:

✓Adesão
✓Invasão
✓Colonização
✓Multiplicação dentro do hospedeiro
✓Evasão do sistema imune hospedeiro

Aperfeiçoamento em Bioinformática

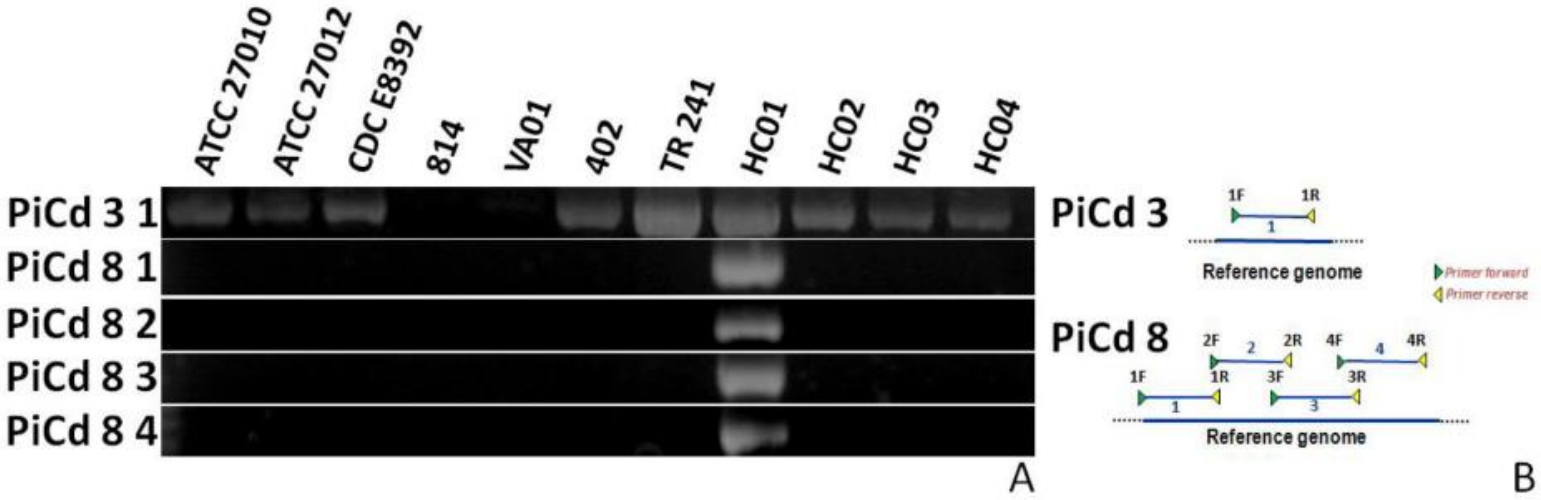


Figure 1. A. Electrophoresis gel exhibiting amplification patterns of PiCds 3 and 8. **B.** Graphic representation of primer annealing. PiCd 3 an PiCd 8 were amplified using 1 and 4 sets of primers, respectively.

GMR Genetics and Molecular Research
Online Journal
ISSN:1676-5680

Short Communication

Plasticity of *Corynebacterium diphtheriae* pathogenicity islands revealed by PCR

S.C. Soares[1], F.A. Dorella[1], L.G.C. Pacheco[2], R. Hirata Jr.[3], A.L. Mattos-Guaraldi[3], V. Azevedo[1] and A. Miyoshi[1]

[1]Departamento de Biologia Geral, Instituto de Ciências Biológicas, Universidade Federal de Minas Gerais, Belo Horizonte, MG, Brasil
[2]Departamento de Biointeração, Universidade Federal da Bahia, Salvador, BA, Brasil
[3]Faculdade de Ciências Médicas, Universidade do Estado do Rio de Janeiro, Rio de Janeiro, RJ, Brasil

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Graduação
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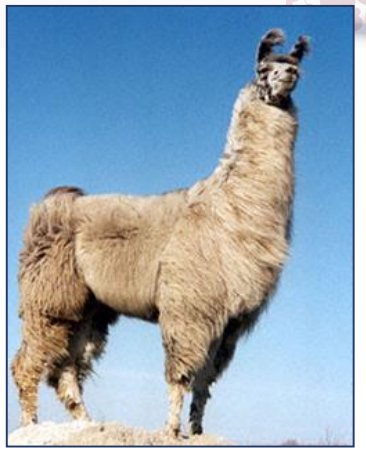
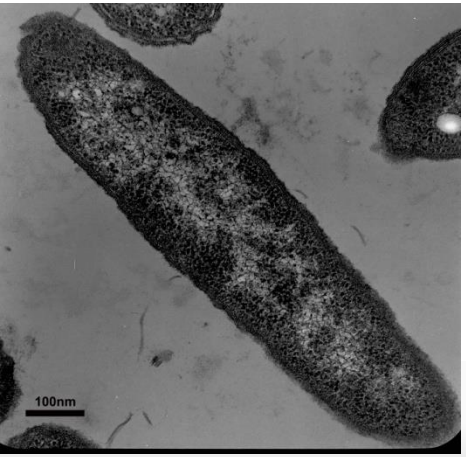
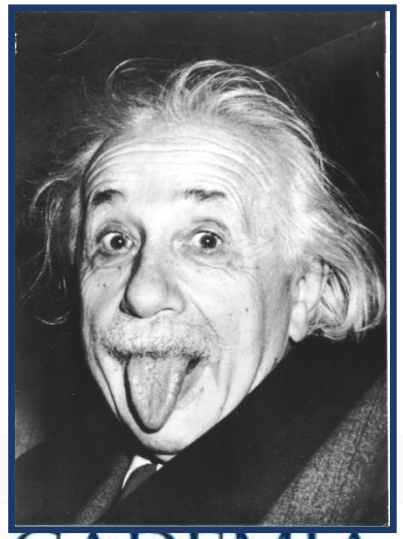
Aperfeiçoamento

Mestrado em Genética







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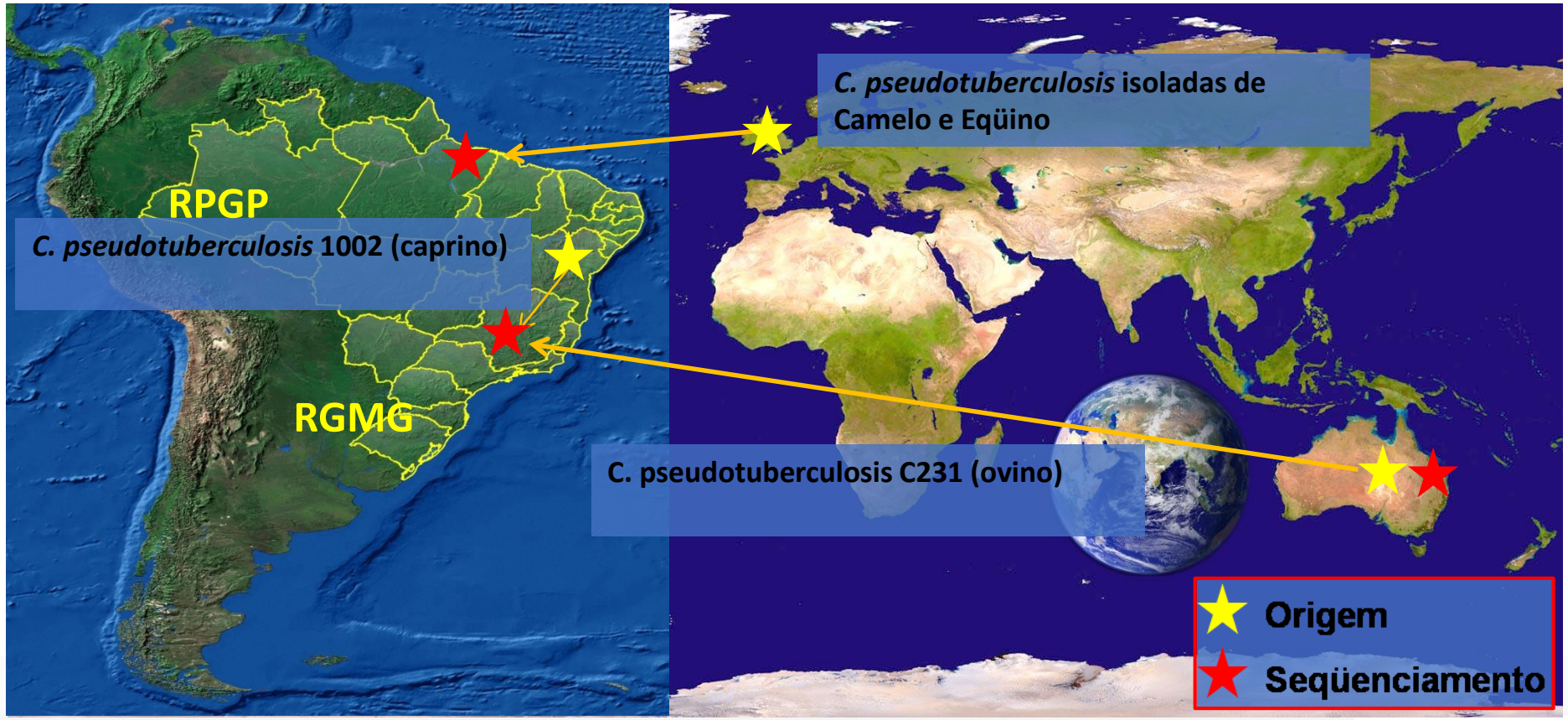

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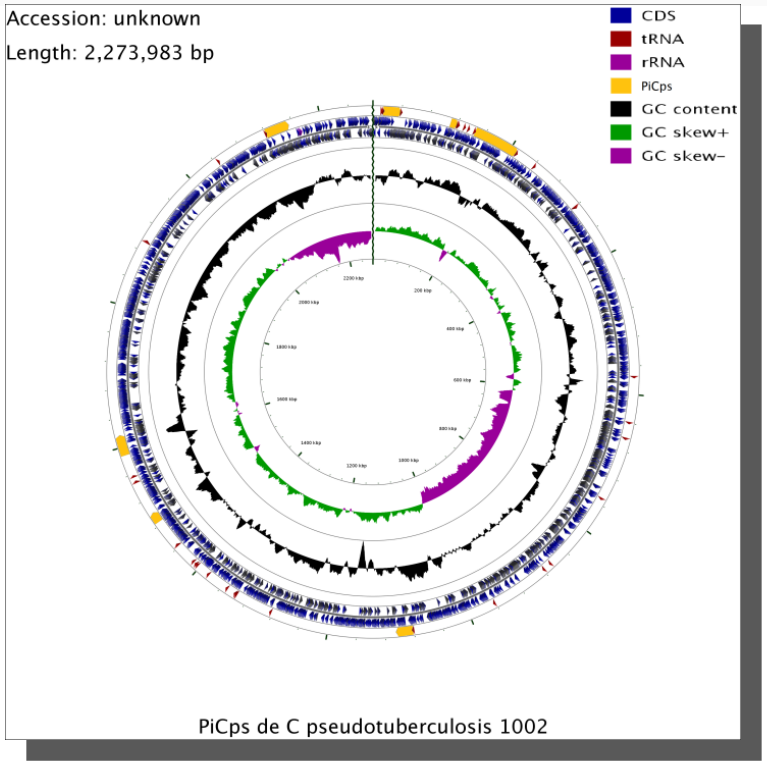
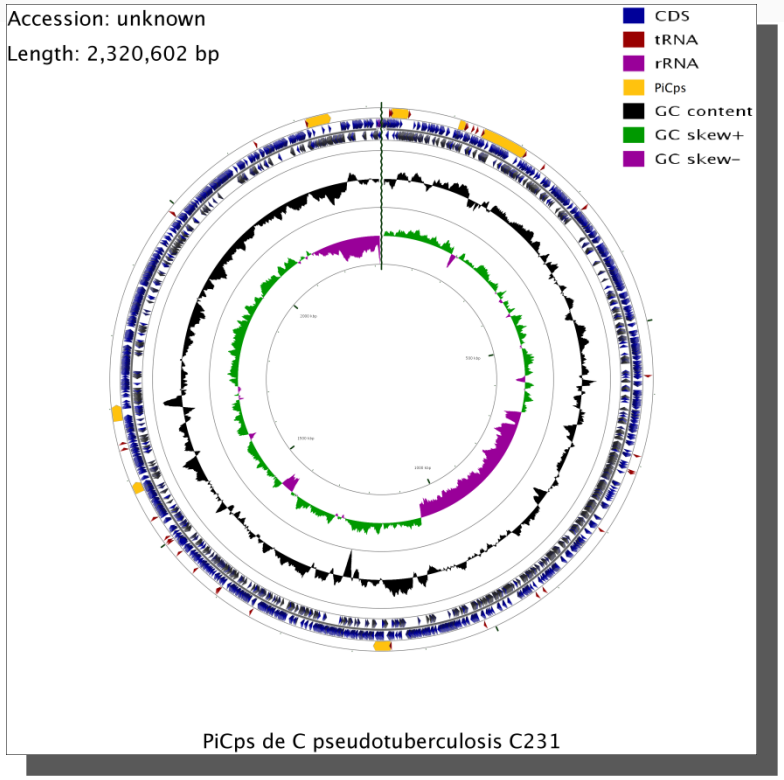


PiCps de C pseudotuberculosis 1002



PiCps de C pseudotuberculosis C231

OPEN ACCESS Freely available online PLoS one

Evidence for Reductive Genome Evolution and Lateral Acquisition of Virulence Functions in Two *Corynebacterium pseudotuberculosis* Strains

Jerônimo C. Ruiz[1,9], Vívian D'Afonseca[2,9], Artur Silva[3], Amjad Ali[2], Anne C. Pinto[2], Anderson R. Santos[2], Aryanne A. M. C. Rocha[2], Débora O. Lopes[4], Fernanda A. Dorella[2], Luis G. C. Pacheco[2,20], Marcília P. Costa[5], Meritxell Z. Turk[2], Núbia Seyffert[2], Pablo M. R. O. Moraes[2], Siomar C. Soares[2], Sintia S. Almeida[2], Thiago L. P. Castro[2], Vinicius A. C. Abreu[2], Eva Trost[6], Jan Baumbach[7], Andreas Tauch[6], Maria Paula C. Schneider[3], John McCulloch[3], Louise T. Cerdeira[3], Rommel T. J. Ramos[3], Adhemar Zerlotini[1], Anderson Dominitini[1], Daniela M. Resende[1,8], Elisângela M. Coser[1], Luciana M. Oliveira[9], André L. Pedrosa[8,10], Carlos U. Vieira[11], Cláudia T. Guimarães[12], Daniela C. Bartholomeu[13], Diana M. Oliveira[5], Fabrício R. Santos[2], Élida Mara Rabelo[14], Francisco P. Lobo[13], Glória R. Franco[13], Ana Flávia Costa[2], Ieso M. Castro[15], Sílvia Regina Costa Dias[14], Jesus A. Ferro[16], José Miguel Ortega[13], Luciano V. Paiva[17], Luiz R. Goulart[11], Juliana Franco Almeida[11], Maria Inês T. Ferro[16], Newton P. Carneiro[12], Paula R. K. Falcão[18], Priscila Grynberg[13], Santuza M. R. Teixeira[13], Sérgio Brommonschenkel[19], Sérgio C. Oliveira[13], Roberto Meyer[20], Robert J. Moore[21], Anderson Miyoshi[2], Guilherme C. Oliveira[1,22], Vasco Azevedo[2,9]

- **Tamanho médio de 2,3 Mb.**
- **~2150 CDSs**
- **598 genes envolvidos na virulência.**
- **Média de conteúdo G+C de ~52.2%**

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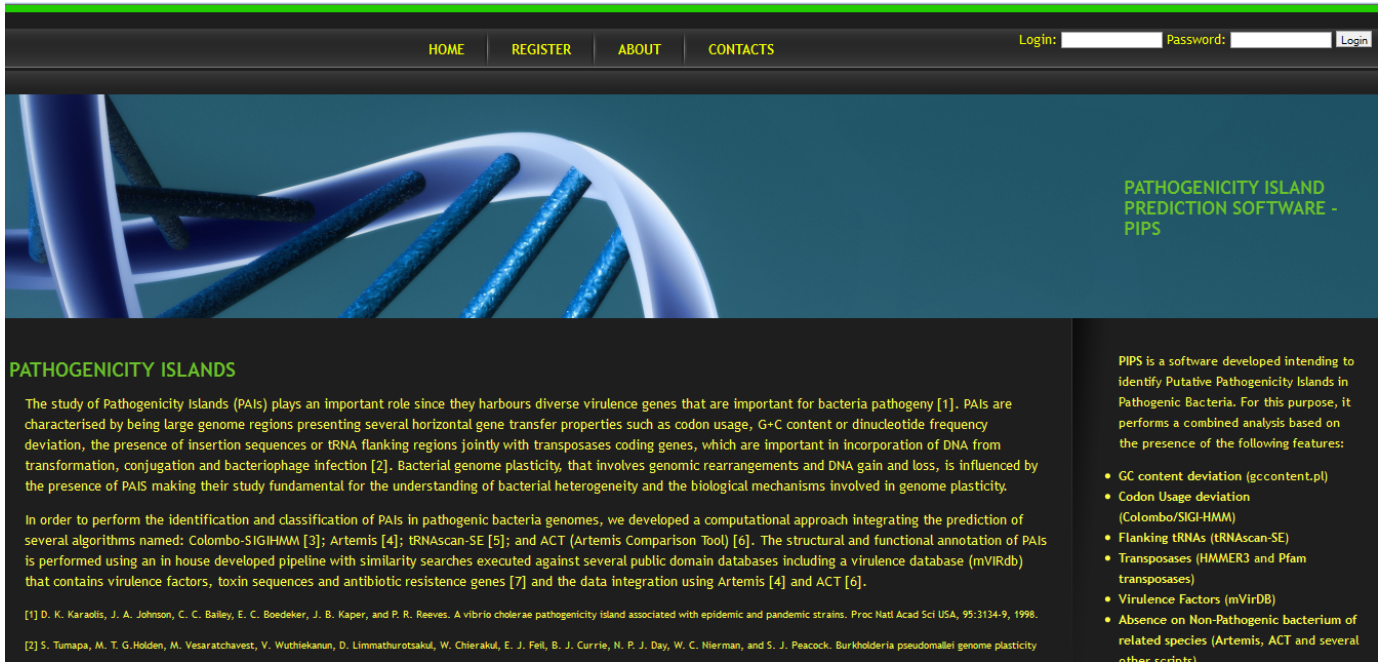
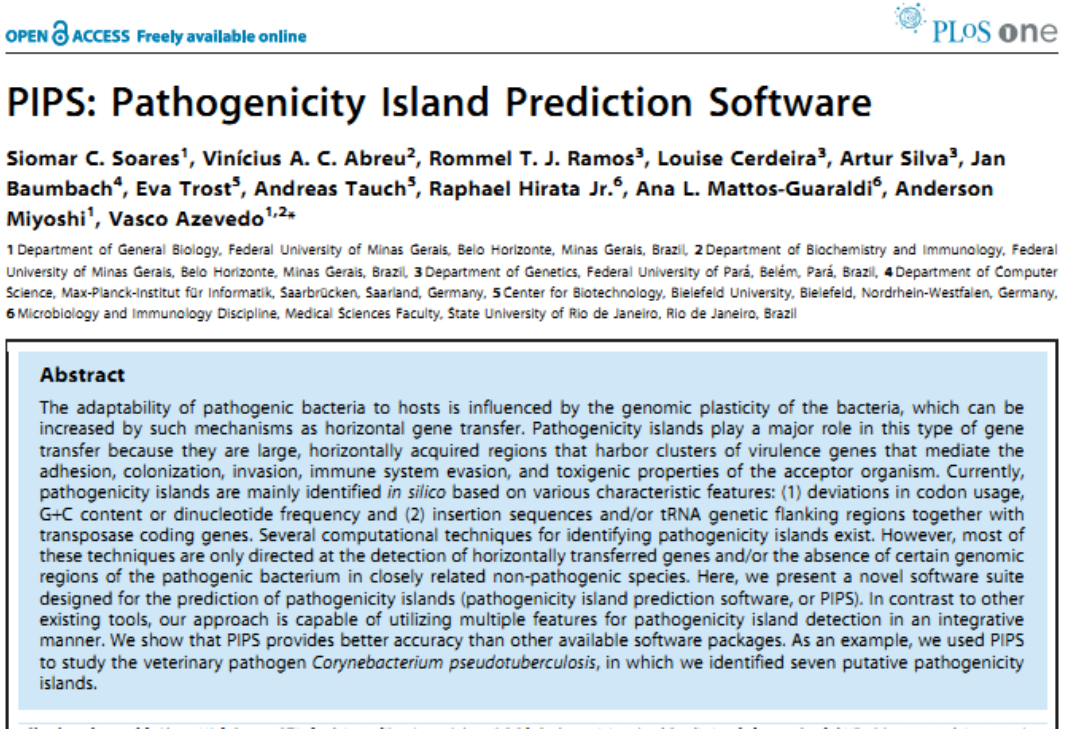
Mestrado em Genética

PIPS: Pathogenicity Island Prediction Software





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PIPS: Pathogenicity Island Prediction Software

Siomar C. Soares[1], Vinícius A. C. Abreu[2], Rommel T. J. Ramos[3], Louise Cerdeira[3], Artur Silva[3], Jan Baumbach[4], Eva Trost[5], Andreas Tauch[5], Raphael Hirata Jr.[6], Ana L. Mattos-Guaraldi[6], Anderson Miyoshi[1], Vasco Azevedo[1,2]*

1 Department of General Biology, Federal University of Minas Gerais, Belo Horizonte, Minas Gerais, Brazil, 2 Department of Biochemistry and Immunology, Federal University of Minas Gerais, Belo Horizonte, Minas Gerais, Brazil, 3 Department of Genetics, Federal University of Pará, Belém, Pará, Brazil, 4 Department of Computer Science, Max-Planck-Institut für Informatik, Saarbrücken, Saarland, Germany, 5 Center for Biotechnology, Bielefeld University, Bielefeld, Nordrhein-Westfalen, Germany, 6 Microbiology and Immunology Discipline, Medical Sciences Faculty, State University of Rio de Janeiro, Rio de Janeiro, Brazil

Abstract

The adaptability of pathogenic bacteria to hosts is influenced by the genomic plasticity of the bacteria, which can be increased by such mechanisms as horizontal gene transfer. Pathogenicity islands play a major role in this type of gene transfer because they are large, horizontally acquired regions that harbor clusters of virulence genes that mediate the adhesion, colonization, invasion, immune system evasion, and toxigenic properties of the acceptor organism. Currently, pathogenicity islands are mainly identified *in silico* based on various characteristic features: (1) deviations in codon usage, G+C content or dinucleotide frequency and (2) insertion sequences and/or tRNA genetic flanking regions together with transposase coding genes. Several computational techniques for identifying pathogenicity islands exist. However, most of these techniques are only directed at the detection of horizontally transferred genes and/or the absence of certain genomic regions of the pathogenic bacterium in closely related non-pathogenic species. Here, we present a novel software suite designed for the prediction of pathogenicity islands (pathogenicity island prediction software, or PIPS). In contrast to other existing tools, our approach is capable of utilizing multiple features for pathogenicity island detection in an integrative manner. We show that PIPS provides better accuracy than other available software packages. As an example, we used PIPS to study the veterinary pathogen *Corynebacterium pseudotuberculosis*, in which we identified seven putative pathogenicity islands.

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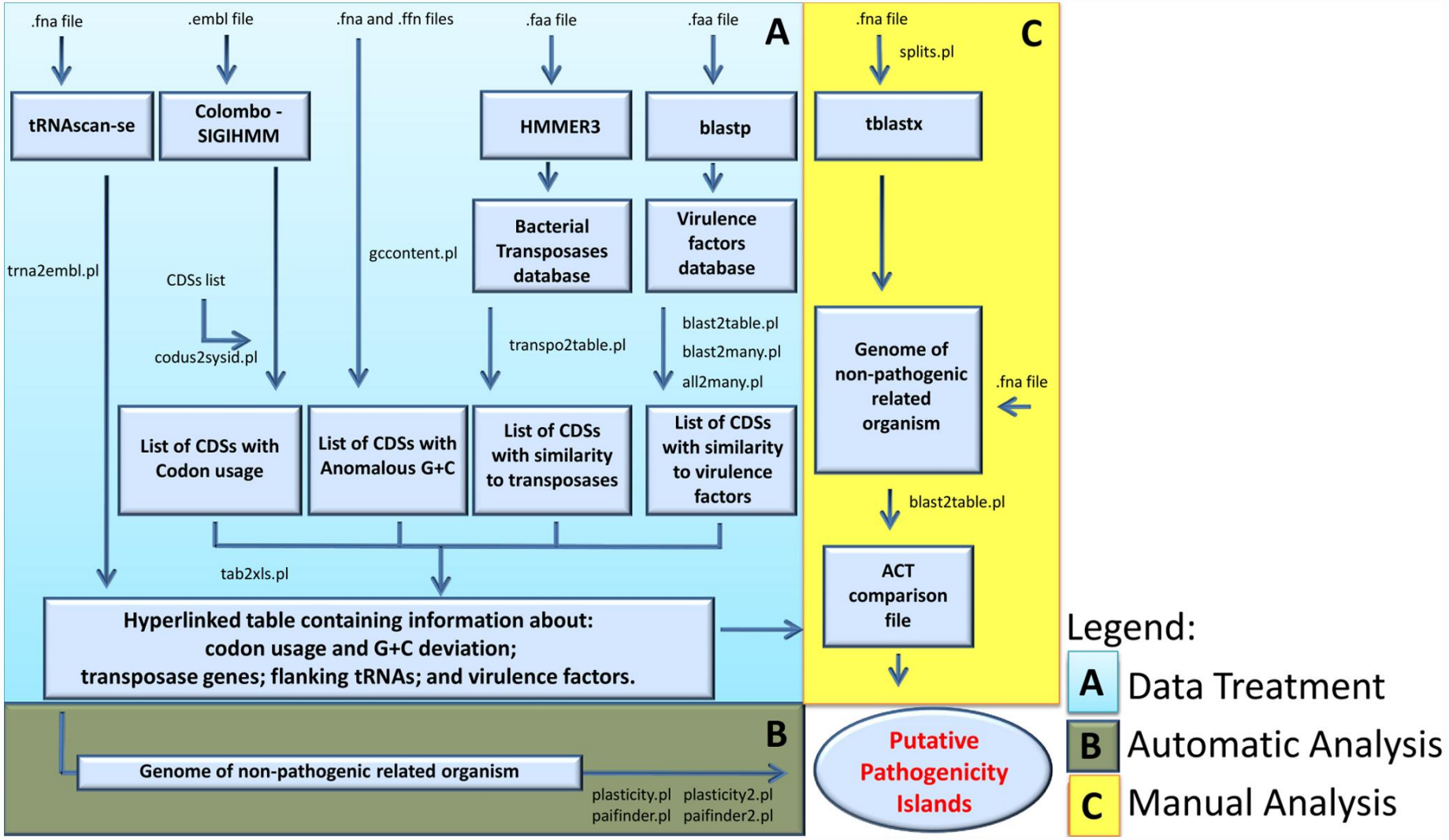

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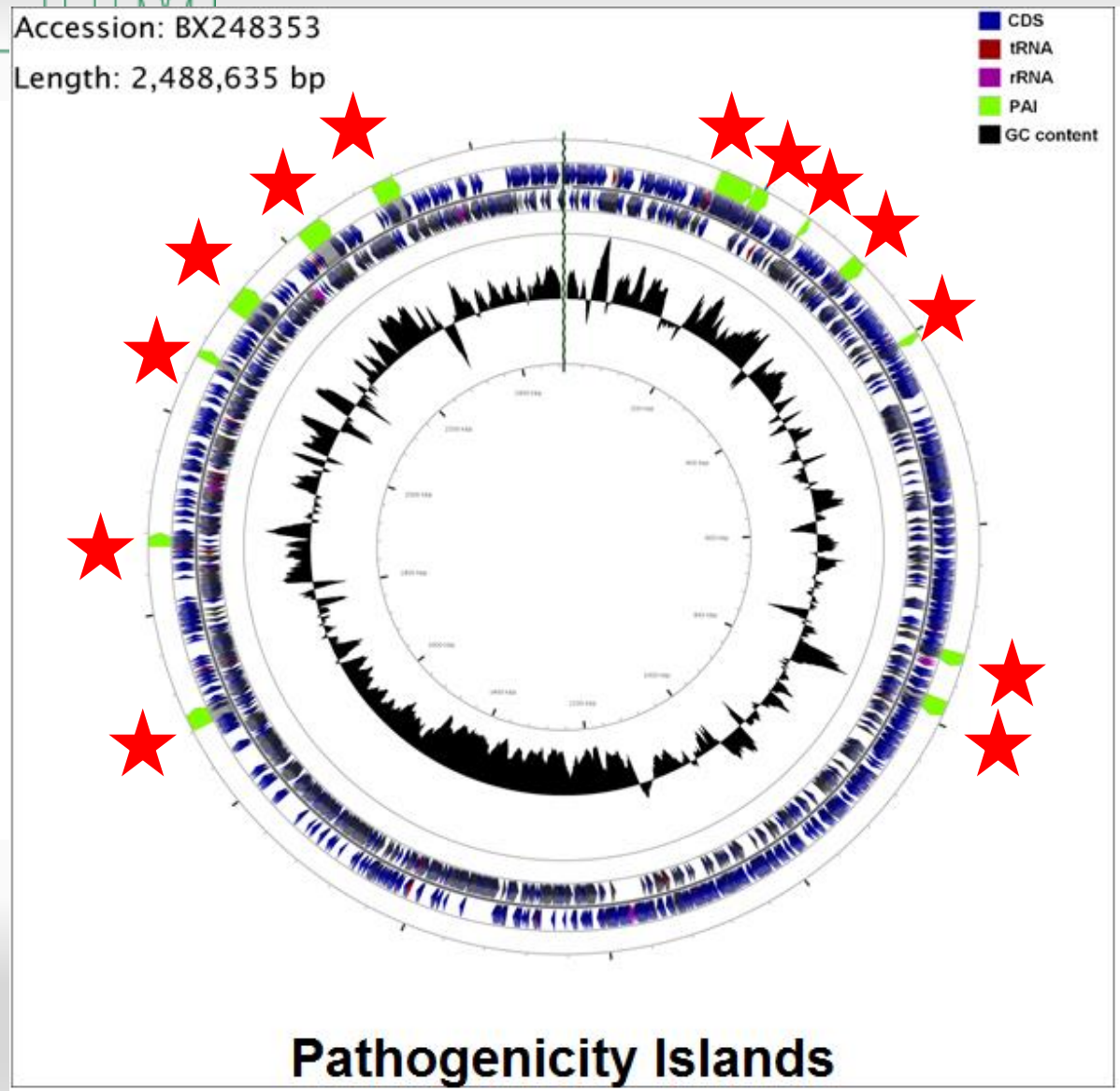
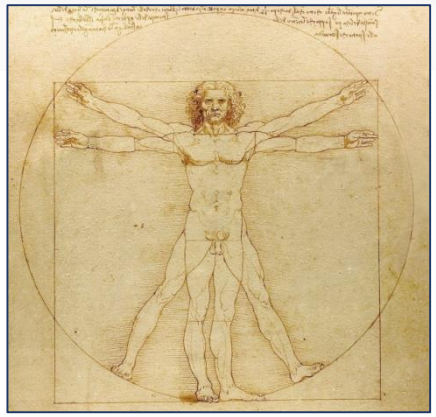
Mestrado em Genética





Corynebacterium diphtheriae

Relatadas na literatura – 13 ilhas de patogenicidade

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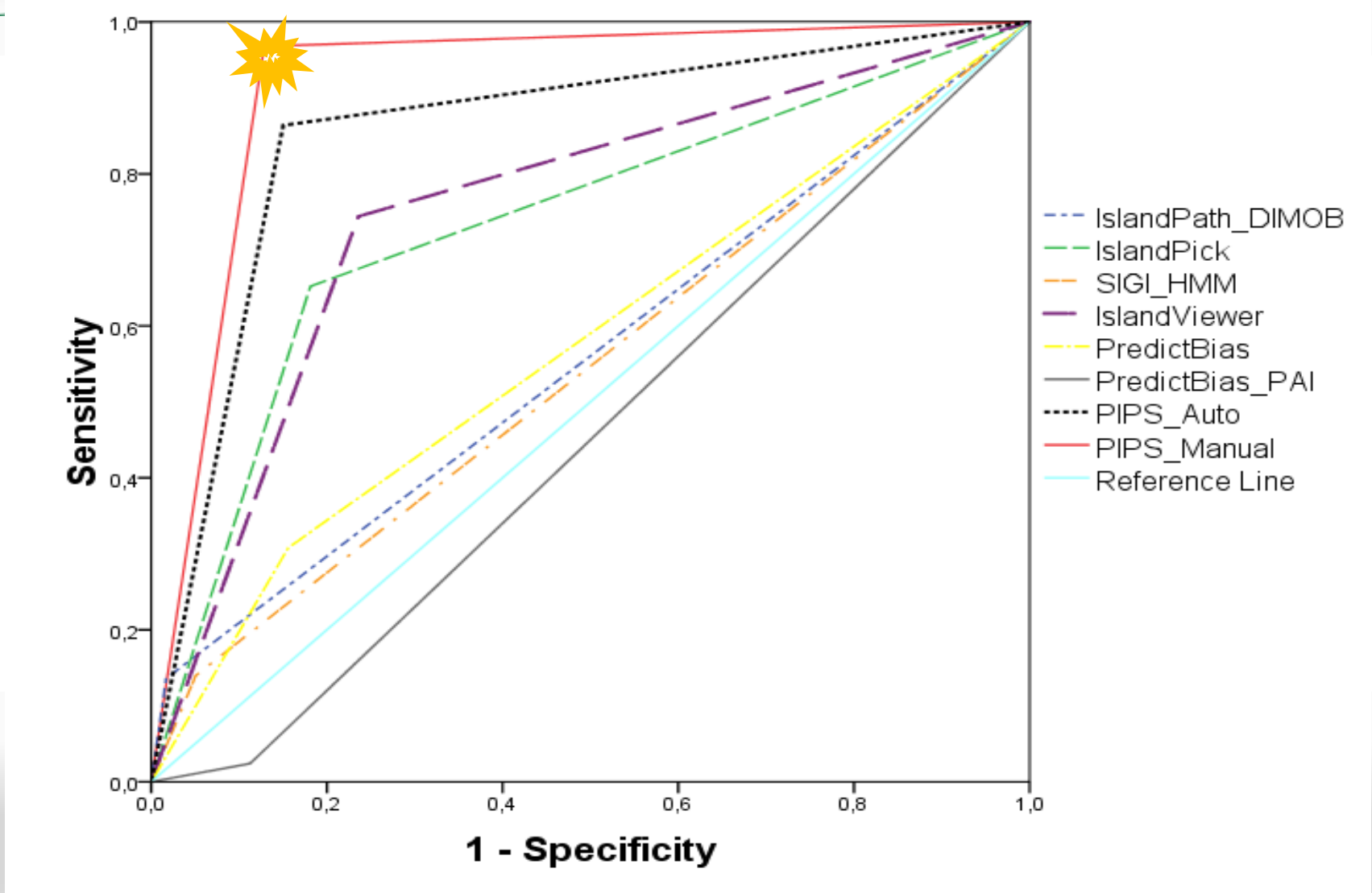

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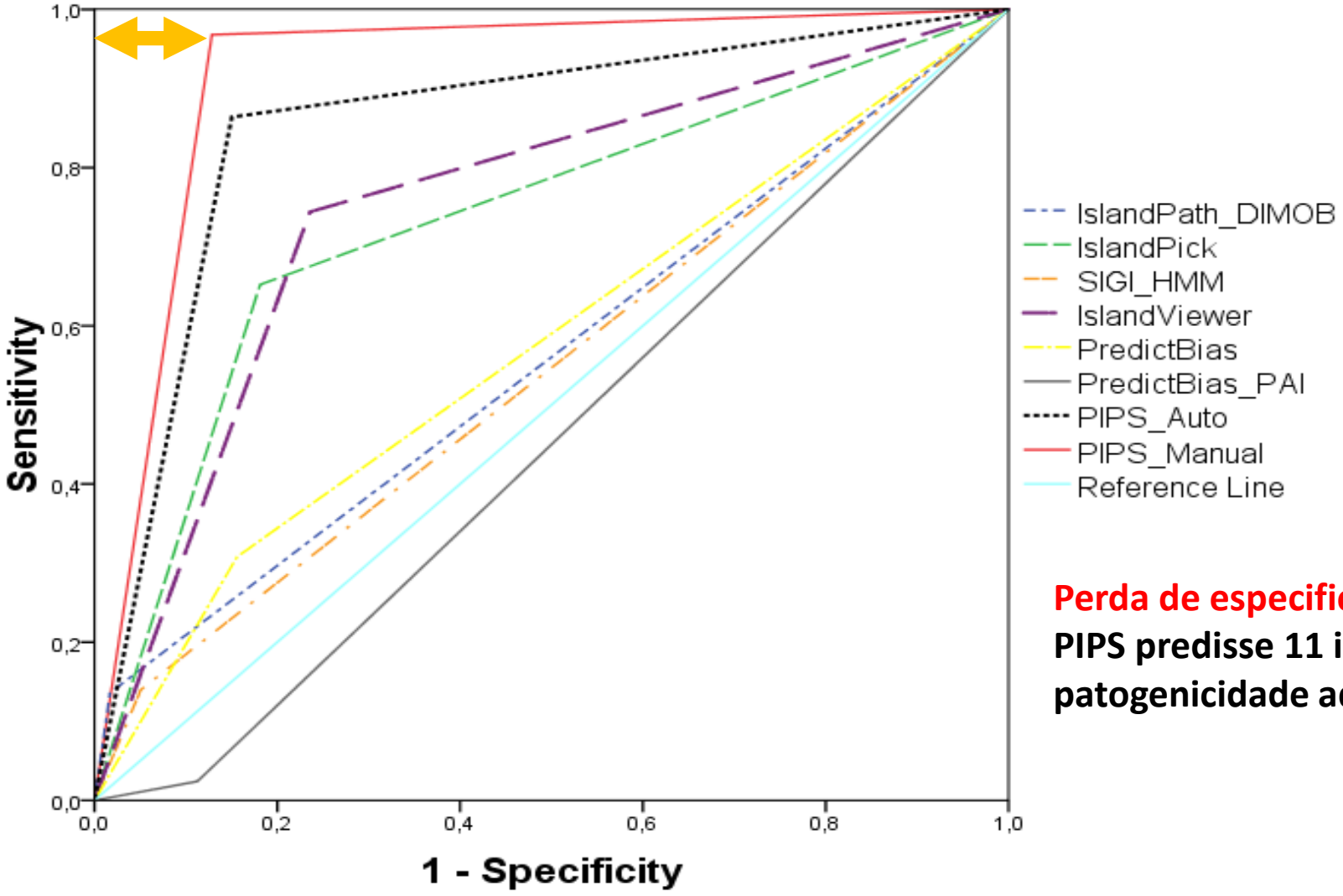
Mestrado em Genética



Perda de especificidade→
PIPS predisse 11 ilhas de patogenicidade adicionais

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	NCTC13129	C7B	PW8	CDCE-8392	31A	241	VA01	HC01	HC02	HC03	HC04	INCA-402	BH8
PICD01	10	6	20	6	2	0	0	0	0	0	0	0	0
PICD02	10	3	3	5	3	5	3	5	5	3	6	5	3
PICD03	10	10	10	10	10	10	10	10	10	10	10	10	10
PICD04	10	4	4	4	3	2	7	2	5	7	8	3	5
PICD05	10	10	10	10	10	10	10	10	10	10	10	10	10
PICD06	10	2	3	3	3	3	7	3	8	6	6	3	4
PICD07	10	1	1	1	1	3	1	3	1	4	1	3	1
PICD08	10	2	2	2	2	8	2	8	2	2	2	3	2
PICD09	10	1	1	1	1	1	1	1	1	1	1	1	4
PICD10	10	0	5	6	0	8	8	8	10	10	20	0	5
PICD11	10	3	2	3	4	7	5	7	7	5	6	2	4
PICD12	10	5	6	6	7	3	6	3	7	6	6	6	3
PICD13	10	1	0	0	0	8	3	8	0	3	4	0	0
PICD14	10	6	3	3	6	5	6	5	5	3	3	4	6
PICD15	10	6	2	6	5	5	6	5	6	6	6	6	5
PICD16	10	10	10	10	10	10	10	10	10	10	10	10	10
PICD17	10	10	10	10	10	10	10	10	10	10	10	10	6
PICD18	10	8	5	5	5	8	6	8	8	6	6	8	10
PICD19	10	7	8	9	9	9	8	9	9	8	7	8	8
PICD20	10	6	8	6	6	10	10	10	10	9	10	6	8
PICD21	10	4	4	3	4	3	3	3	3	3	3	3	4
PICD22	10	4	6	4	4	4	7	4	6	5	20	4	4
PICD23	10	8	8	8	9	8	9	8	9	9	9	8	8
PICD24	10	8	8	7	8	7	7	7	7	6	8	8	8

Legend:

0	0-10%
1	10-20%
2	20-30%
3	30-40%
4	40-50%
5	50-60%
6	50-60%
7	60-70%
8	70-80%
9	80-90%
10	90-100%
20	The whole island is duplicated

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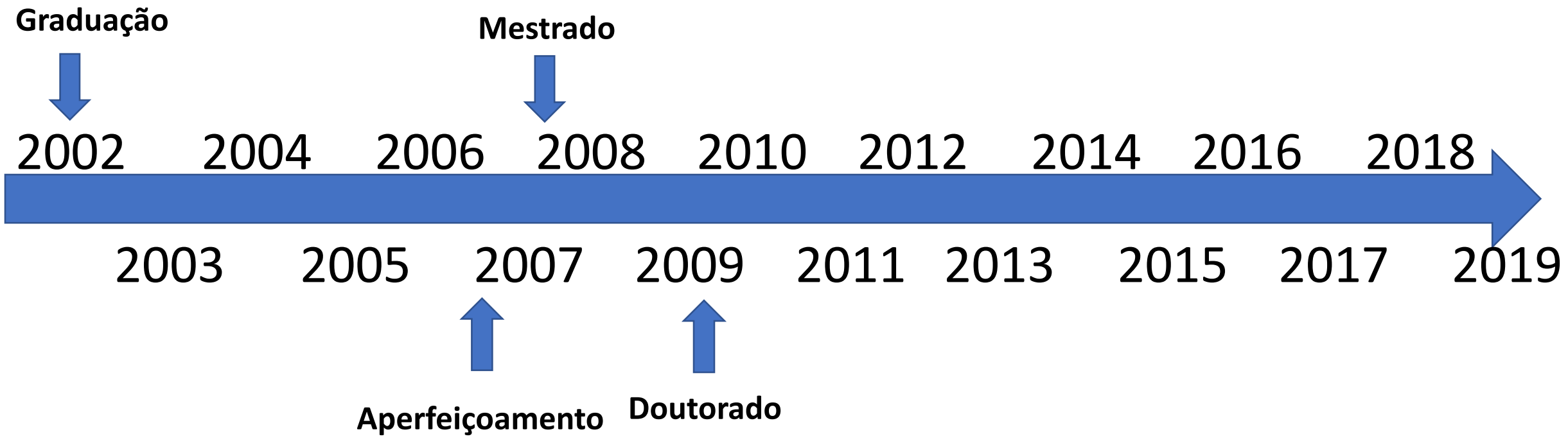
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Aperfeiçoamento
Doutorado

Doutorado em Genética

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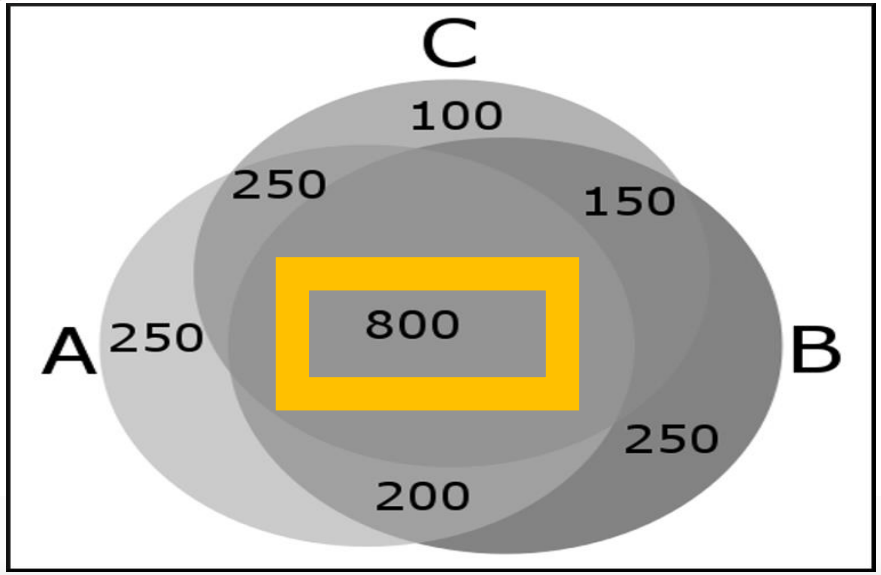
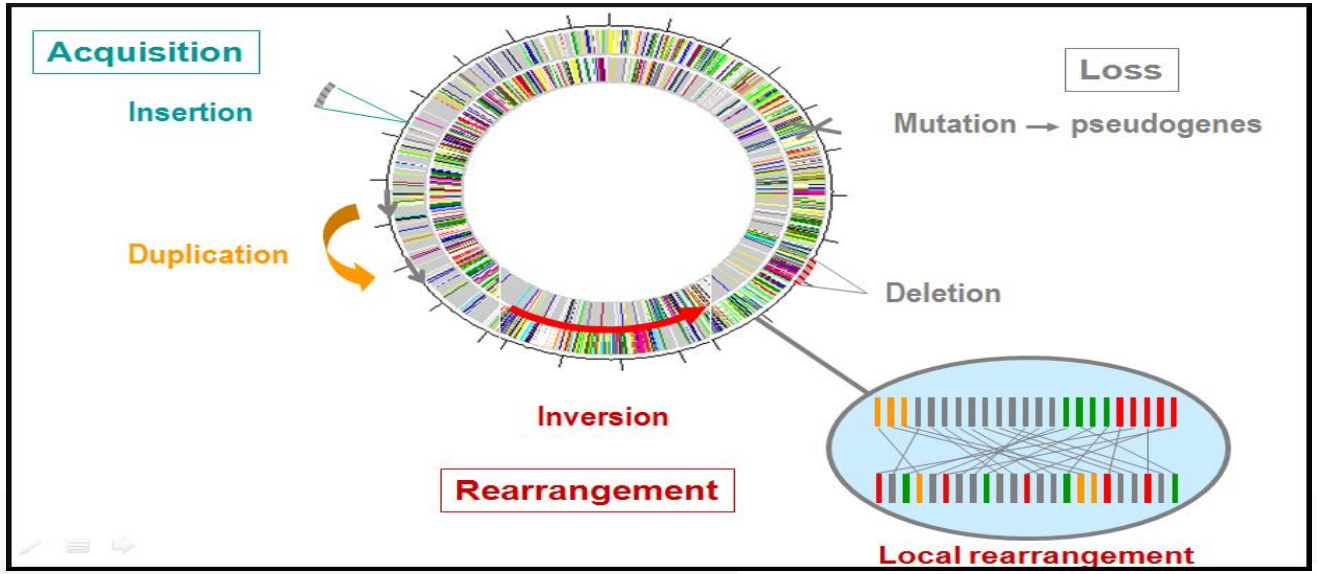
Doutorado em Genética

Pan-genômica é uma área recente da genômica que tem como objetivo principal a comparação genômica entre diferentes linhagens ou espécies bacterianas





Identificar o genoma conservado e os eventos de plasticidade genômica.

Tettelin et al (2005)

Doutorado em Genética

O conjunto de dados completo é representativo de vários hospedeiros com sintomas diversos dos países mais afetados

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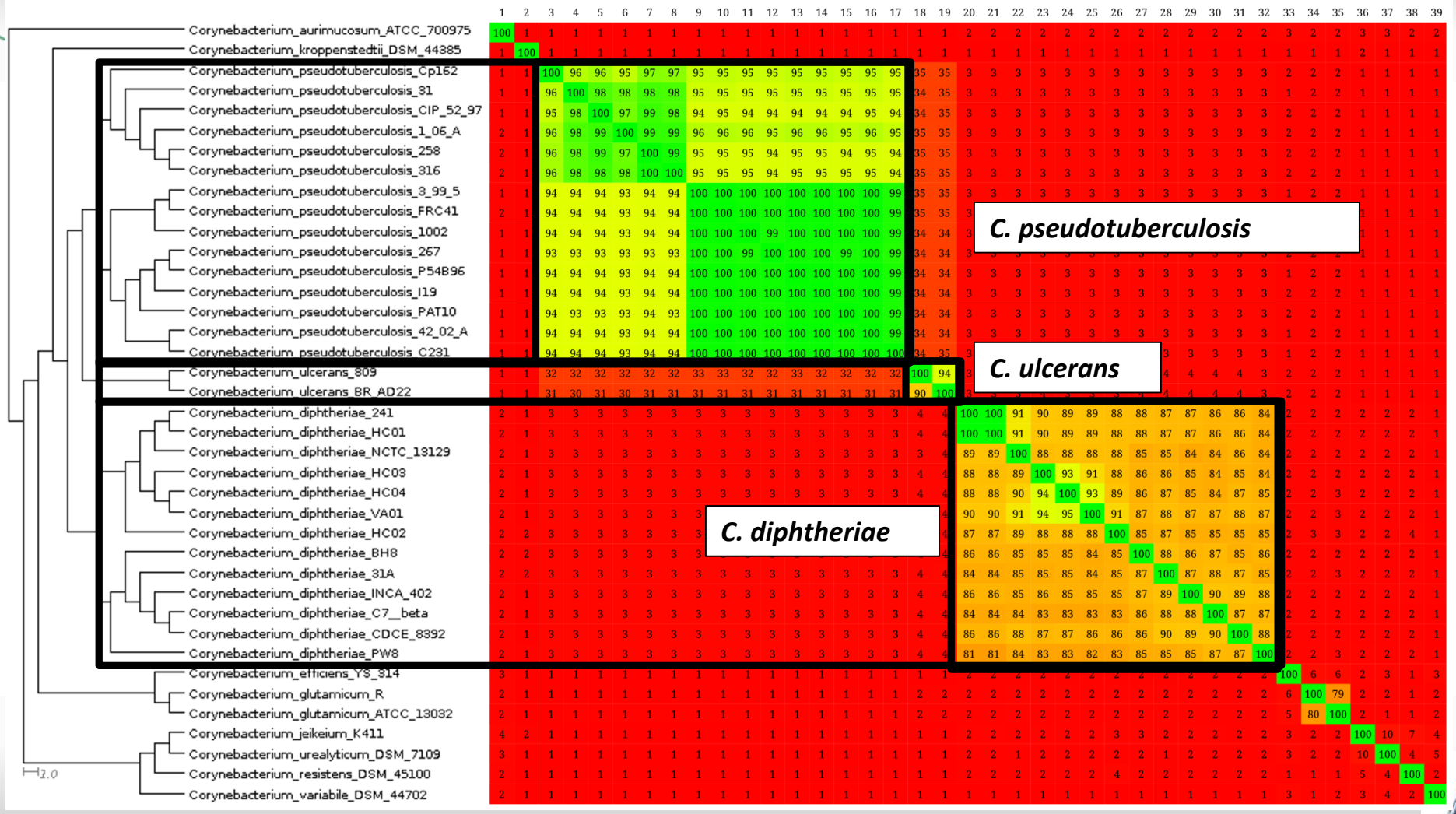

Phylogenomic tree and heatmap analyses of the genus *Corynebacterium*.
Heatmap and phylogenomic tree generated with Gegenees and SplitsTree (using data from Gegenees).

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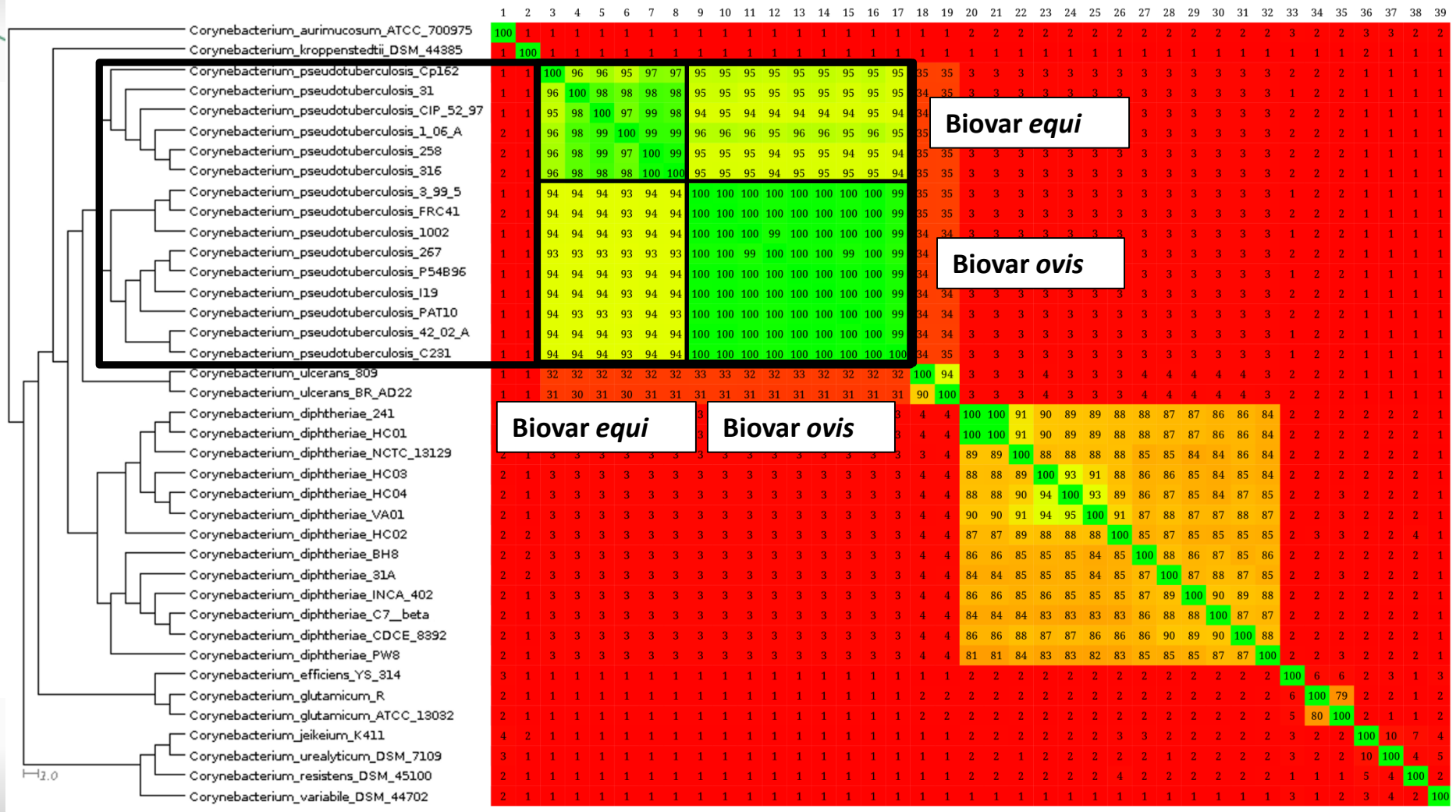
Doutorado em Genética



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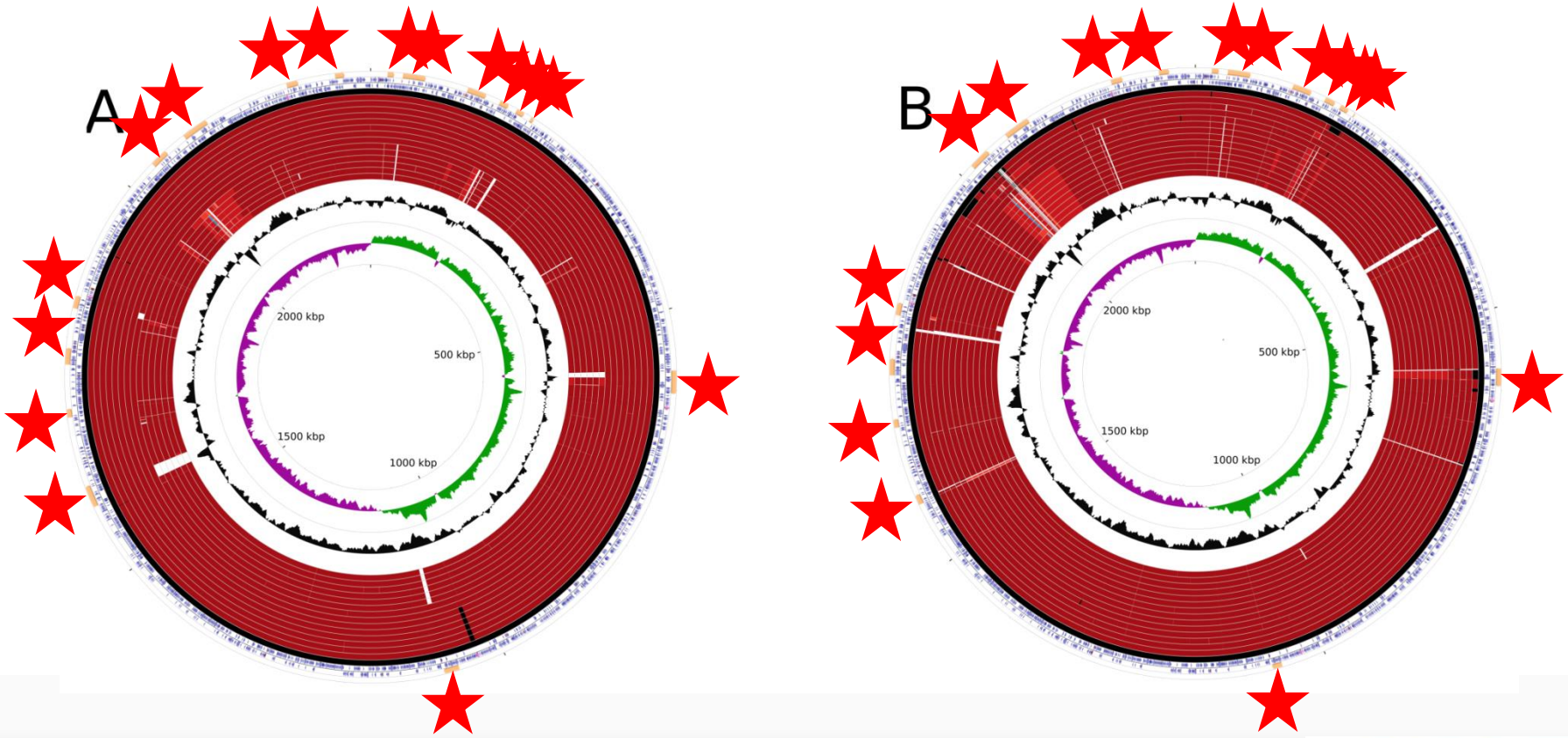

Comparative genomic maps of *C. pseudotuberculosis* biovar *equi* and *ovis* strains.
Figure generated with CCT: CGView Comparison Tool

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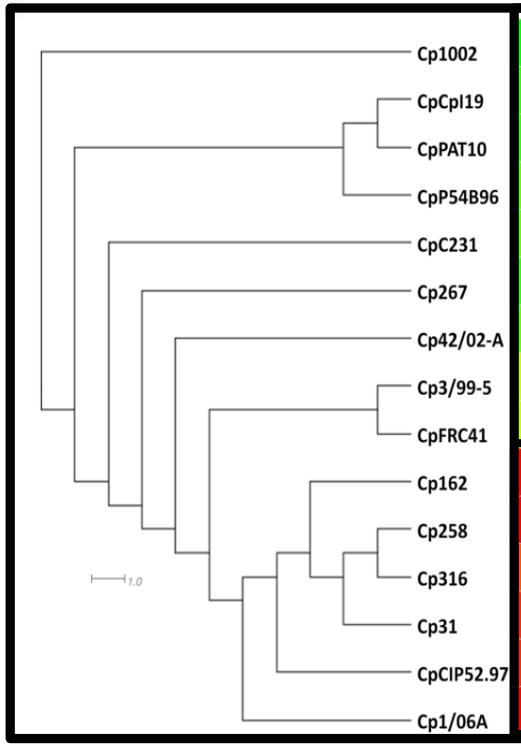

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
Cp1002	100	96	96	96	96	90	96	88	88	86	84	89	88	84	91
CpCpI19	95	100	99	98	97	90	94	86	88	86	84	89	89	83	92
CpPAT10	94	98	100	98	97	89	93	86	88	86	84	88	88	83	91
CpP54B96	94	96	97	100	96	88	92	84	87	85	83	87	87	81	89
CpC231	92	93	94	94	100	87	90	82	85	82	81	84	83	79	87
Cp267	95	94	94	94	96	100	93	89	90	85	83	88	87	82	90
Cp42/02-A	91	90	90	90	90	84	100	87	84	84	83	85	87	82	91
Cp3/99-5	86	86	86	86	84	83	90	100	87	83	84	84	85	78	89
CpFRC41	85	85	86	86	83	82	86	86	100	83	83	84	86	78	87
Cp162	65	66	67	67	65	63	68	63	67	100	83	80	84	78	85
Cp258	66	68	68	68	67	64	71	67	70	85	100	85	87	82	85
Cp316	70	72	72	72	70	69	74	67	72	87	87	100	88	84	88
Cp31	68	69	70	70	68	66	73	66	71	87	85	84	100	79	86
CpCIP52.97	68	69	69	69	69	65	72	64	68	85	85	86	85	100	87
Cp1/06A	65	67	67	66	65	62	71	65	67	81	79	79	81	77	100

Biovar *ovis*

Biovar *equi*

Biovar *ovis*

Biovar *equi*

Phylogenomic tree and heatmap analyses of *Corynebacterium pseudotuberculosis* strains created based on plasticity of pathogenicity islands.
Identification of putative PAIs was performed with PIPS: Pathogenicity Island Prediction Tool. Plasticity was assessed from data generated by Edgar. Phylogenomic tree was created by SplitsTree with data from plasticity analyses.

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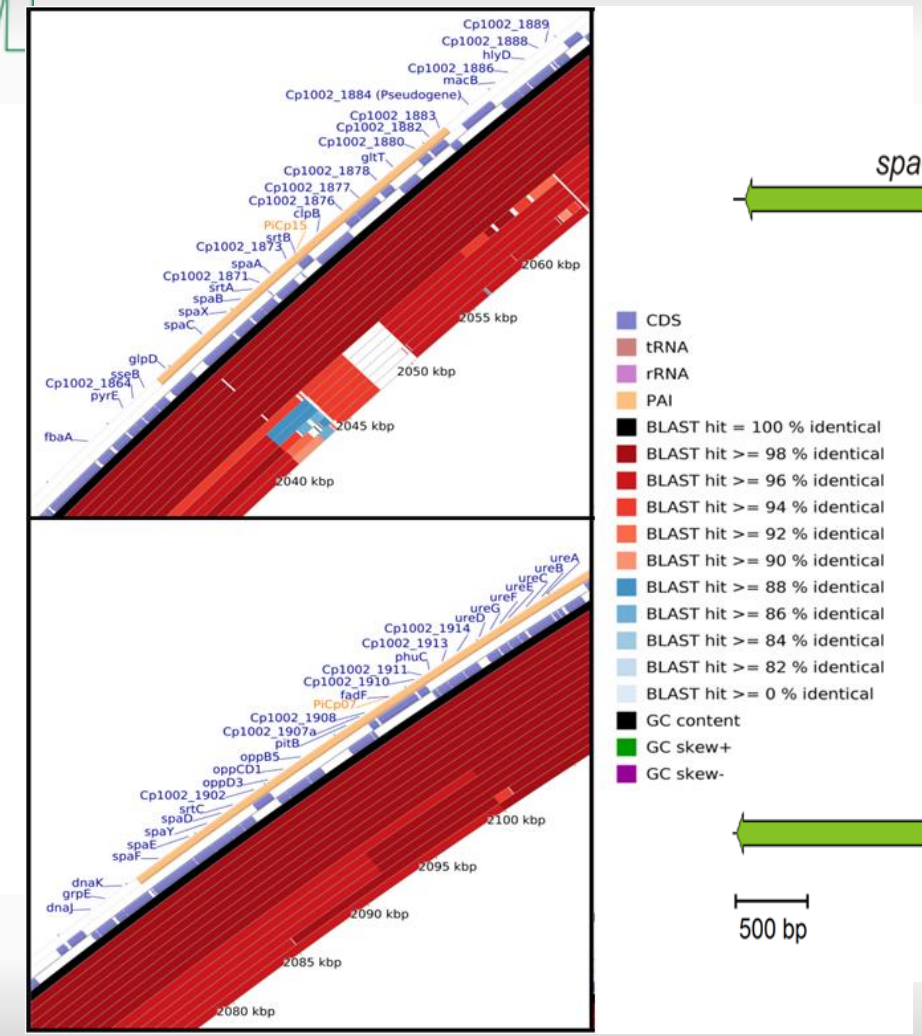

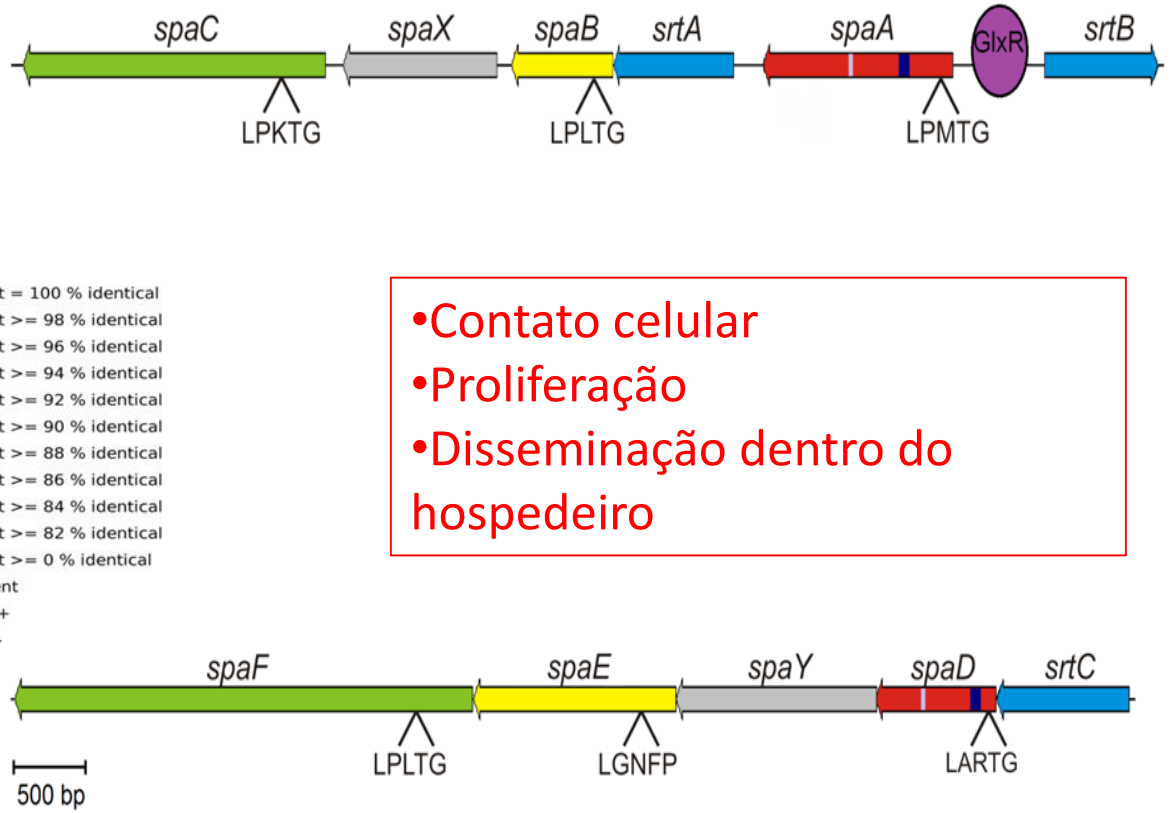

- Contato celular
- Proliferação
- Disseminação dentro do hospedeiro

Figure . Plasticity of pili clusters of genes, *spaA* and *spaD*, in *C. pseudotuberculosis*.

Gene regions encoding adhesive pili of *C. pseudotuberculosis* FRC41.
Figure from Trost *et al.* (2012).

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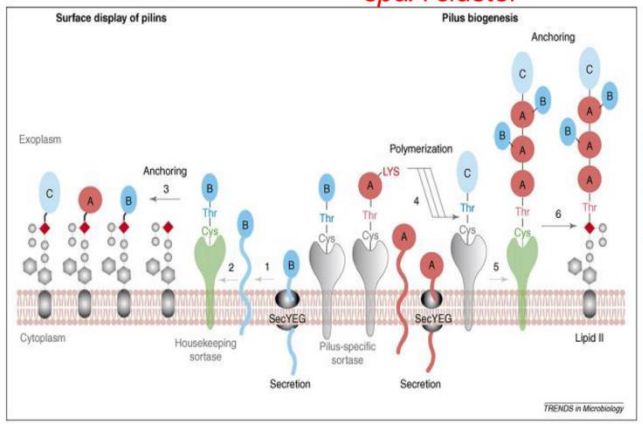
Doutorado em Genética

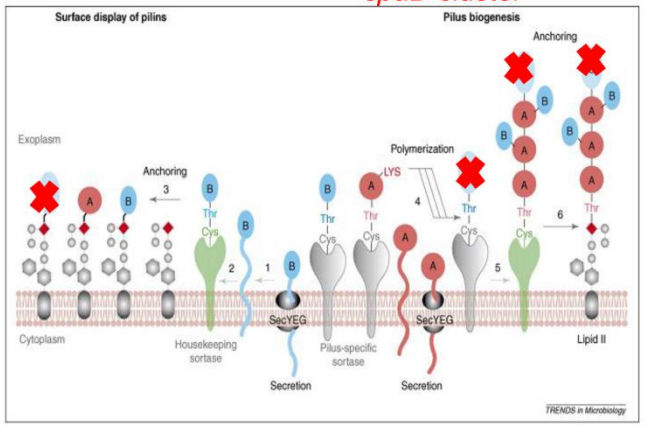
spaA cluster



bv. *ovis*

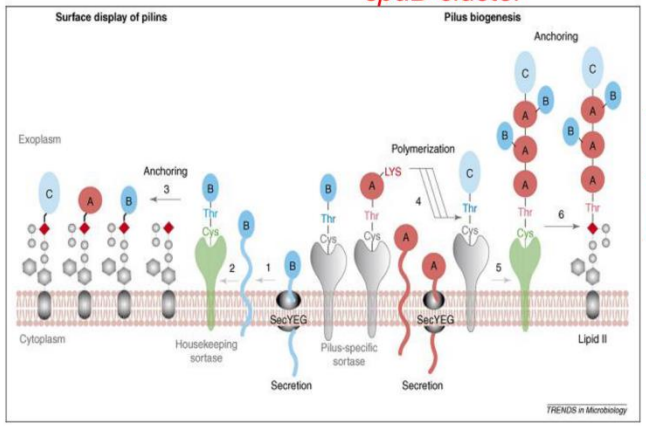
Completo

spaD cluster



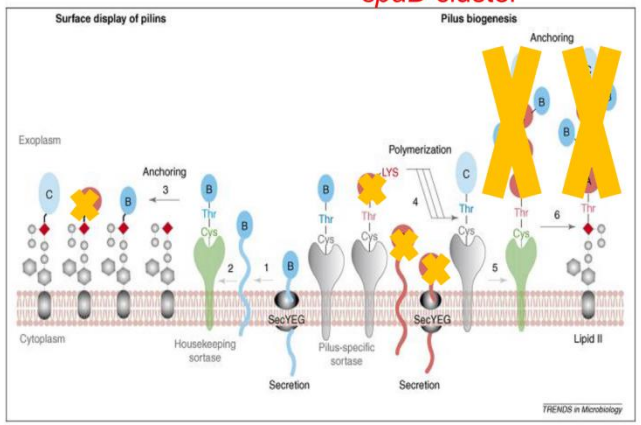
Frameshift no tip pilin

spaD cluster



Completo

spaD cluster

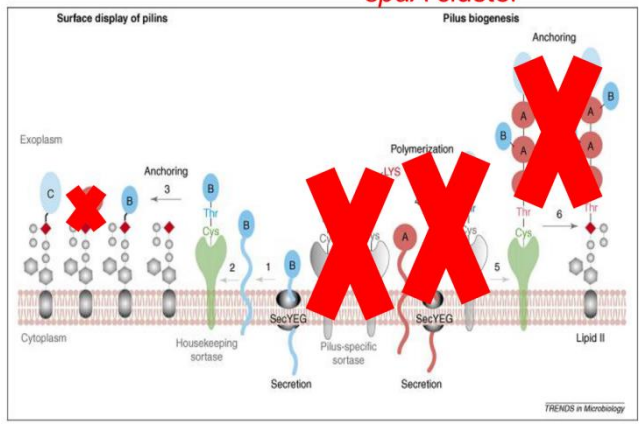


Frameshift na major pilin

Figure from Mandlik *et al*. (2008)

Doutorado em Genética

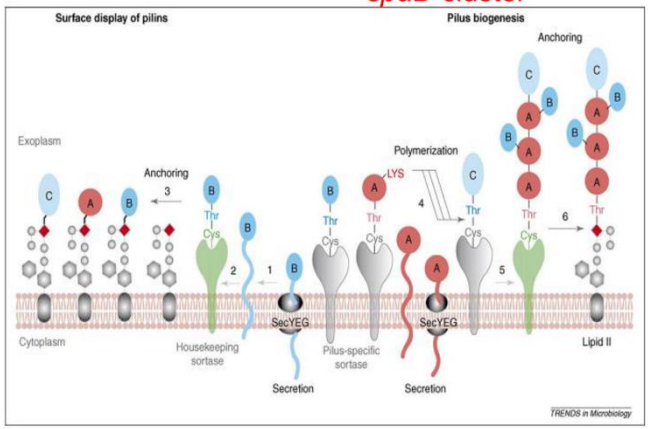
spaA cluster



bv. *equi*

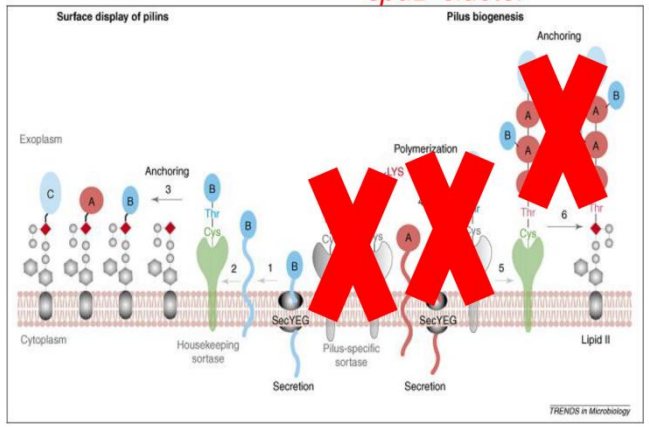
sortase específica e o major pilin estão deletados

spaD cluster



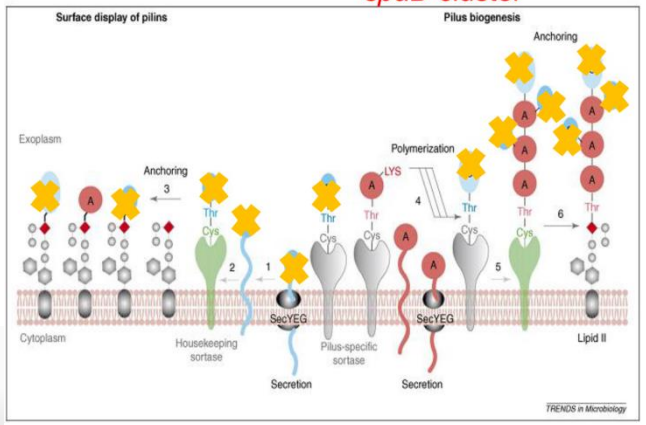
Completo

spaD cluster



Frameshift na sortase específica

spaD cluster



Base e tip pilin estão unidas na mesma matriz de leitura

Figure from Mandlik *et al*. (2008)

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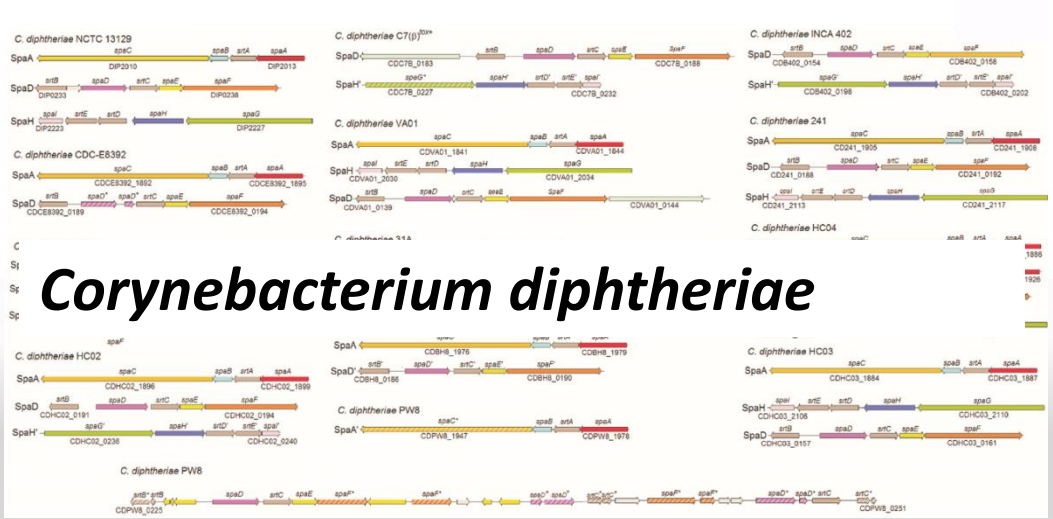
Doutorado em Genética

bv. *equi*

- **Pili tem um papel importante na adesão e internalização;**
- **Em *C. diphtheriae*, somente linhagens invasivas apresentam um conjunto completo de genes de pili;**
- **Acometimento visceral pelo biovar *equi* é raro;**
- **As linhagens do Biovar *equi* são altamente variáveis no cluster de genes de pili.**



Corynebacterium diphtheriae

Poderia a formação de pili estar relacionada aos padrões específicos da doença, ie, acometimentos visceral e superficial?

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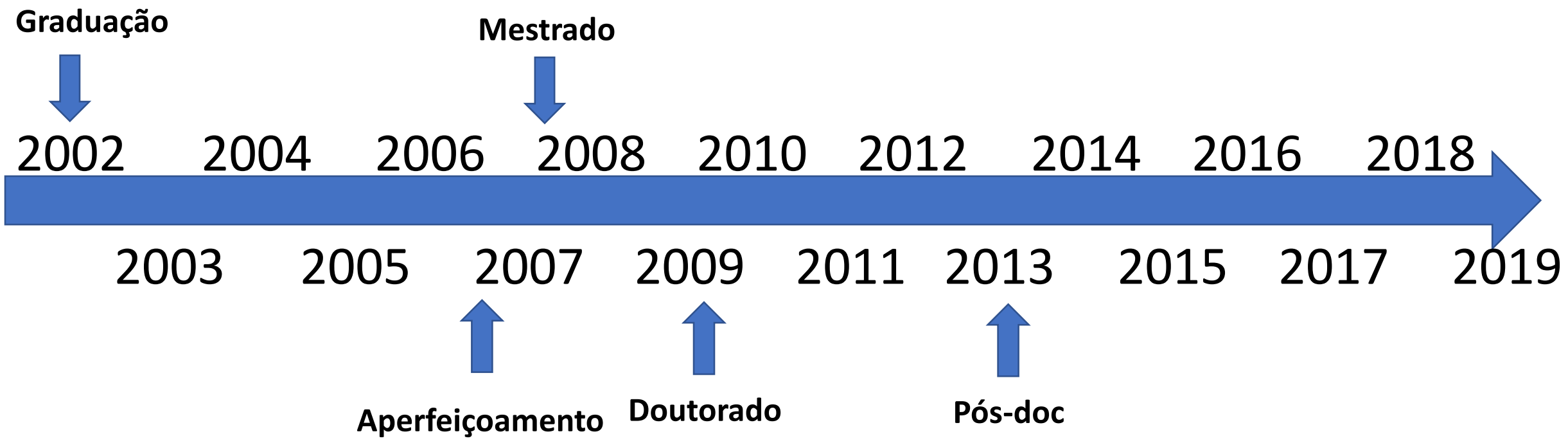
Graduação
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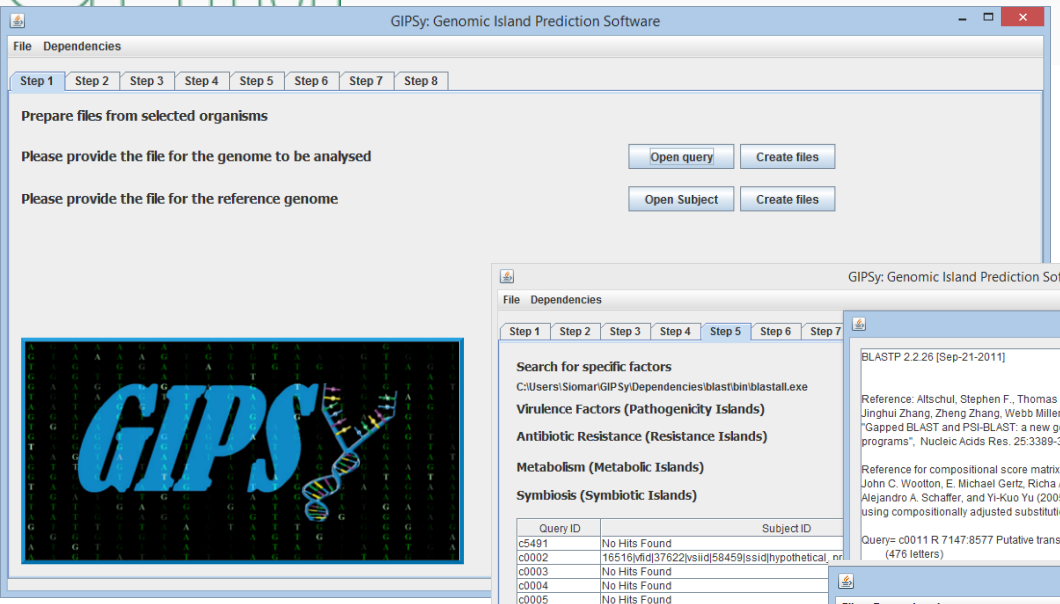
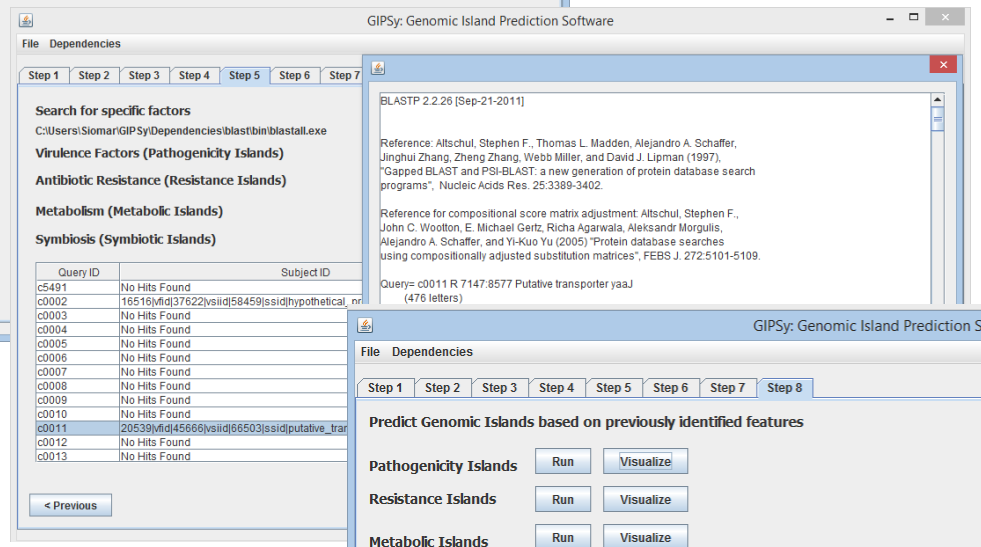
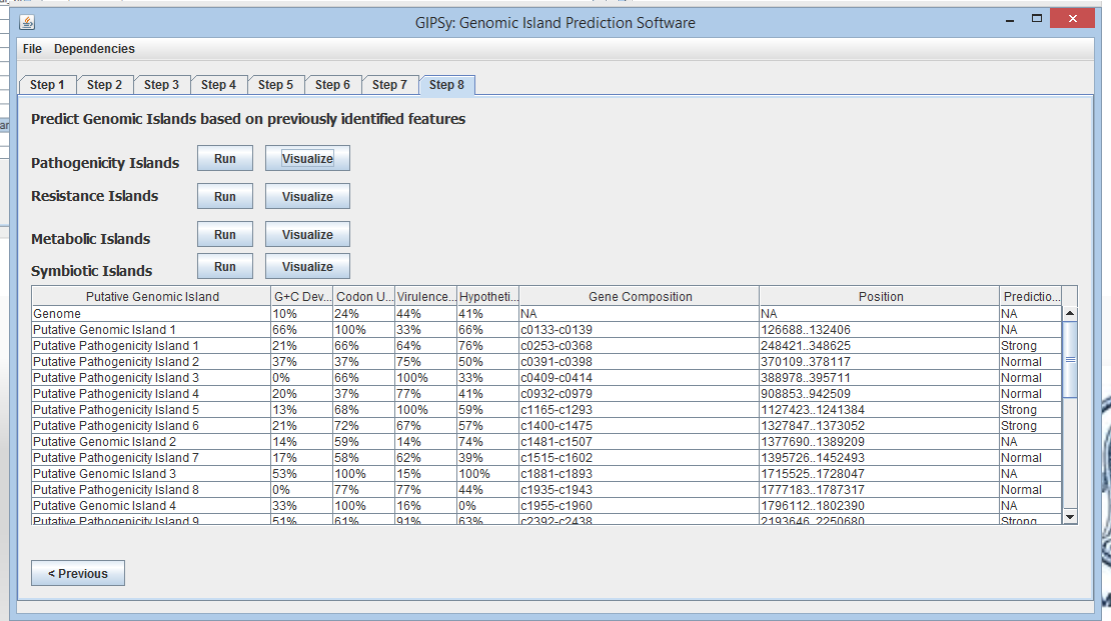
Aperfeiçoamento
Doutorado
Pós-doc

Pós-doutorado



- **Atualiza a metodologia do PIPS para a predição de todas as classes de ilhas genômicas**





Putative Genomic Island	G+C Dev...	Codon U...	Virulence...	Hypotheti...	Gene Composition	Position	Predictio...
Genome	10%	24%	44%	41%	NA	NA	NA
Putative Genomic Island 1	66%	100%	33%	66%	c0133-c0139	126688..132406	NA
Putative Pathogenicity Island 1	21%	66%	64%	76%	c0253-c0368	248421..348625	Strong
Putative Pathogenicity Island 2	37%	37%	75%	50%	c0391-c0398	370109..378117	Normal
Putative Pathogenicity Island 3	0%	66%	100%	33%	c0409-c0414	388978..395711	Normal
Putative Pathogenicity Island 4	20%	37%	77%	41%	c0932-c0979	908853..942509	Normal
Putative Pathogenicity Island 5	13%	68%	100%	59%	c1165-c1293	1127423..1241384	Strong
Putative Pathogenicity Island 6	21%	72%	67%	57%	c1400-c1475	1327847..1373052	Strong
Putative Genomic Island 2	14%	59%	14%	74%	c1481-c1507	1377690..1389209	NA
Putative Pathogenicity Island 7	17%	58%	62%	39%	c1515-c1602	1395726..1452493	Normal
Putative Genomic Island 3	53%	100%	15%	100%	c1881-c1893	1715525..1728047	NA
Putative Pathogenicity Island 8	0%	77%	77%	44%	c1935-c1943	1777183..1787317	Normal
Putative Genomic Island 4	33%	100%	16%	0%	c1955-c1960	1796112..1802390	NA
Putative Pathogenicity Island 9	51%	61%	91%	63%	c2392-c2438	2193646..2250680	Strong

- **Interface gráfica baseada em Java**
- **Compatível com Windows e Linux**

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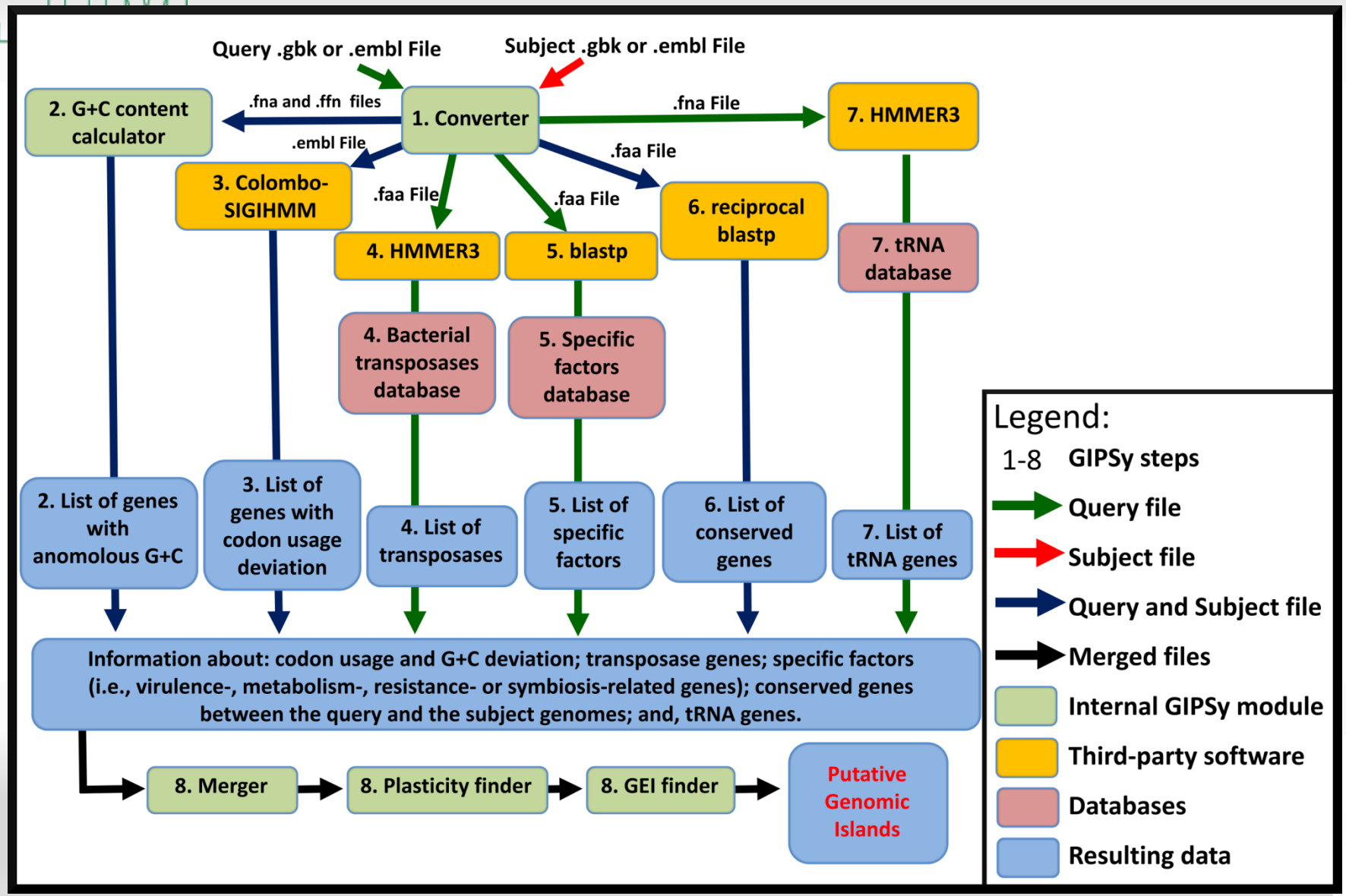
Pós-doutorado



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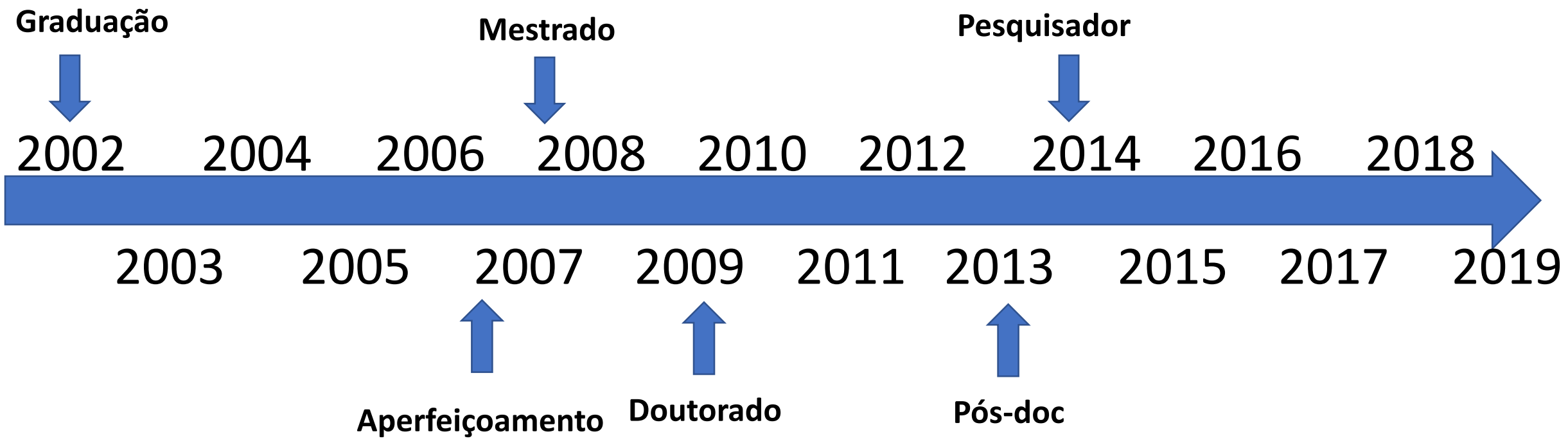
Graduação
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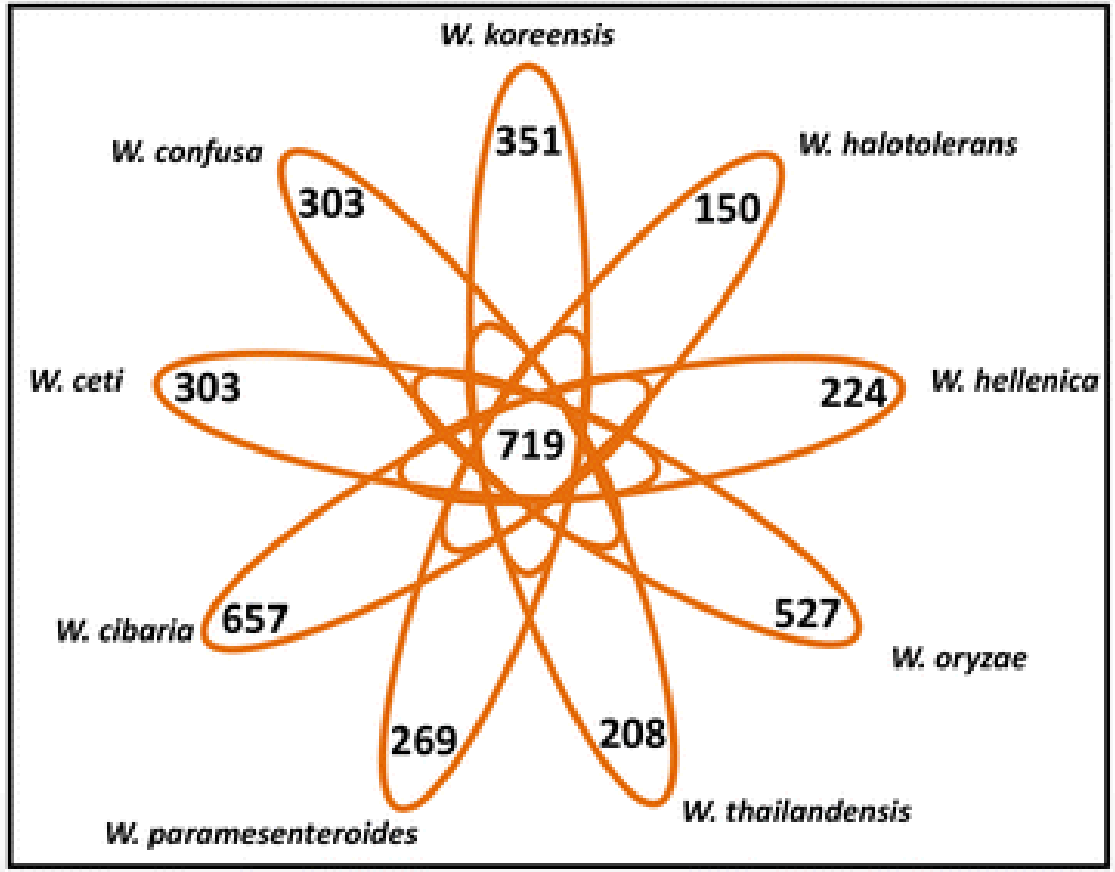
Aperfeiçoamento
Doutorado
Pós-doc

Laboratório oficial do Ministério da Pesca



Weissela ceti

Figueiredo *et al. BMC Genomics* (2015) 16:1095
DOI 10.1186/s12864-015-2324-4

BMC Genomics

RESEARCH ARTICLE Open Access

Comparative genome analysis of *Weissella ceti*, an emerging pathogen of farm-raised rainbow trout

Henrique C. P. Figueiredo[1,3*], Siomar C. Soares[1], Felipe L. Pereira[1], Fernanda A. Dorella[1], Alex F. Carvalho[1], Júnia P. Teixeira[1], Vasco A. C. Azevedo[2] and Carlos A. G. Leal[1]

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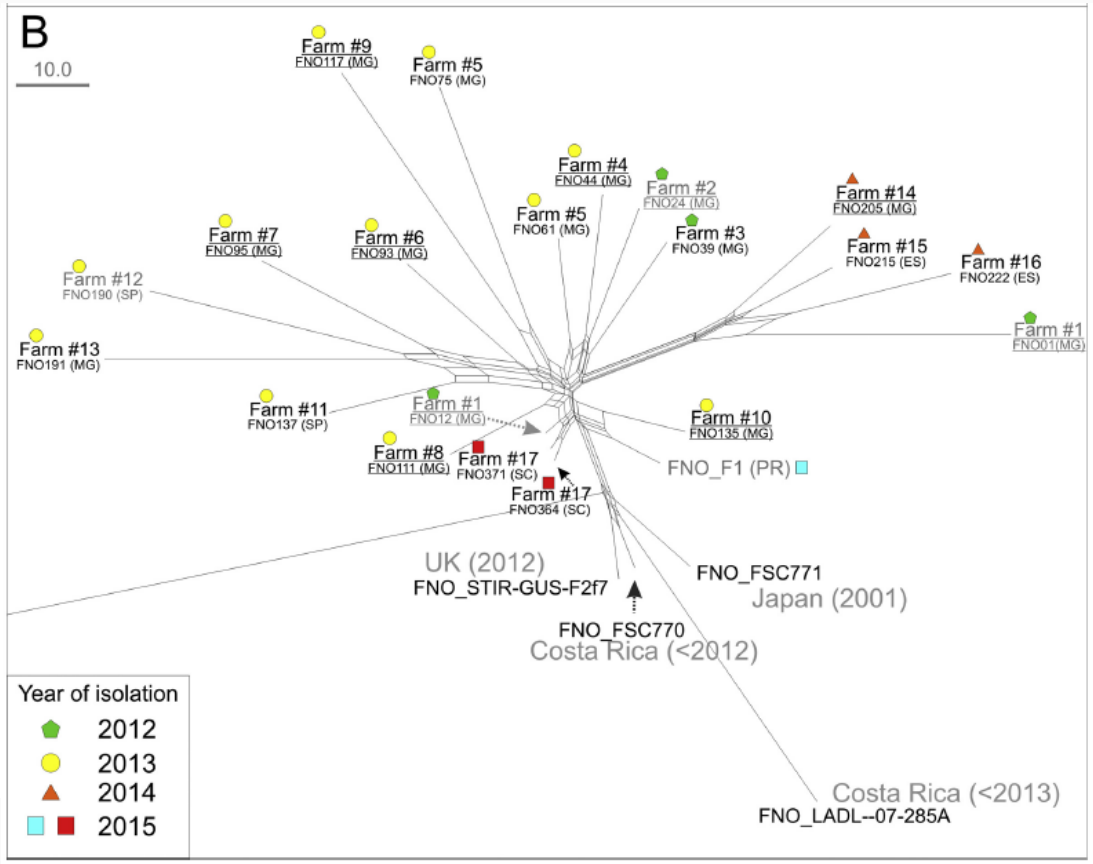
MCMXVI

Laboratório oficial do Ministério da Pesca



ARTICLE IN PRESS

Genomics xxx (xxxx) xxx–xxx

Contents lists available at ScienceDirect

Genomics

journal homepage: www.elsevier.com/locate/ygeno

Complete genome sequencing of sixteen *Francisella noatunensis* subsp. *orientalis* isolates: A genomic approach for molecular characterization and spread dynamics of this clonal population

Felipe Luiz Pereira[a,1], Lucas Amorim Gonçalves[a,b,1], Guilherme Campos Tavares[a], Siomar de Castro Soares[c], Fernanda Alves Dorella[a], Alex Fiorini de Carvalho[a], Márcia Pimenta Leibowitz[a], Carlos Augusto Gomes Leal[a], Vasco Ariston de Carvalho Azevedo[b], Henrique César Pereira Figueiredo[a,*]

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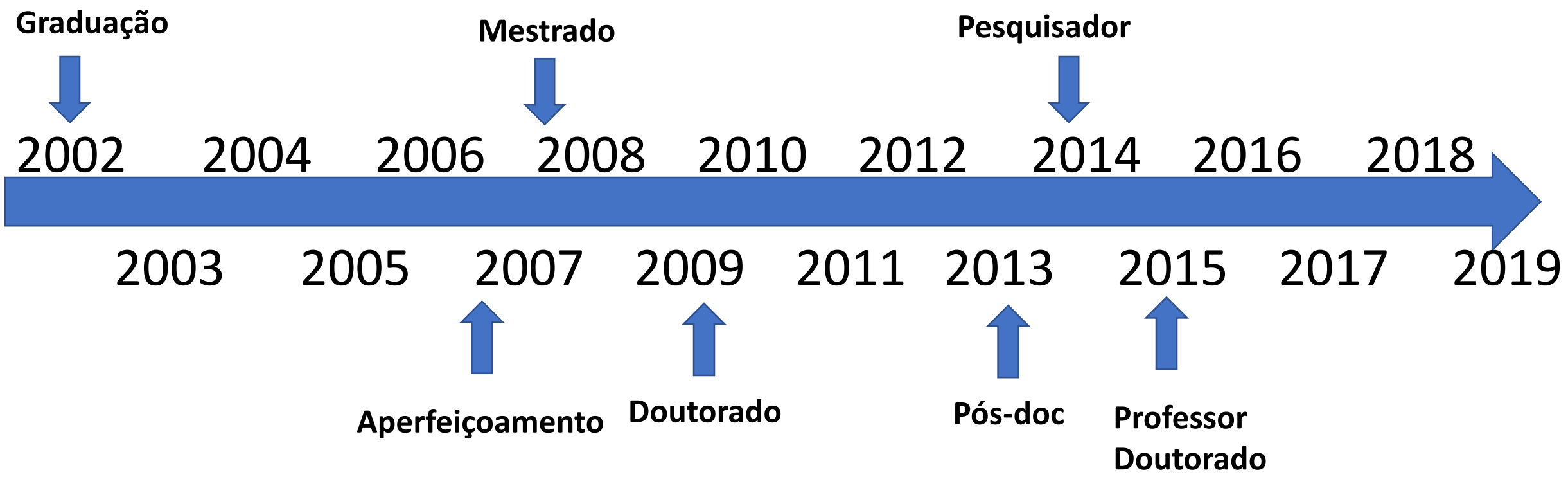
Graduação
Mestrado
Pesquisador
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2017
2019
Aperfeiçoamento
Doutorado
Pós-doc
Professor
Doutorado

UFTM

UFTM

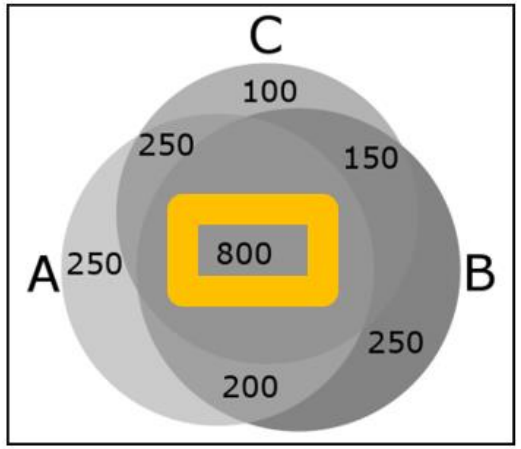
Graduação – 28

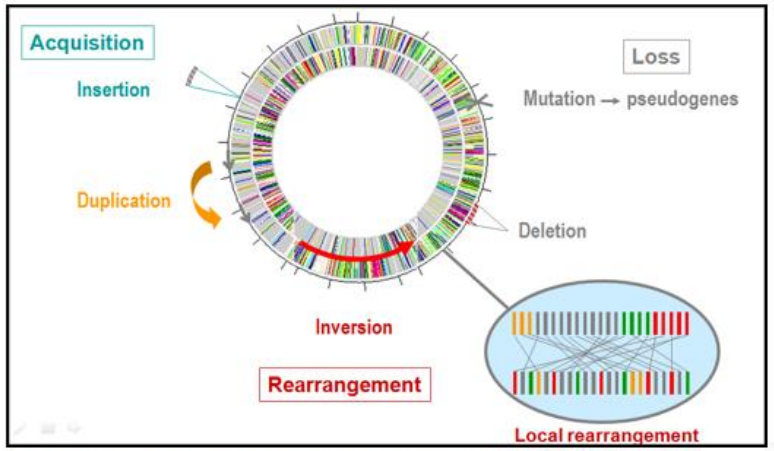
Pós-graduação - 19

Alvo efetivo

- **Vital para o patógeno (*ambas)**
- Não homólogo ao hospedeiro (*ambas)
- Proteínas do exoproteoma, membrana celular (*vacinologia reversa)
- Resposta imune adaptativa (*vacinologia reversa)
- Proteínas citoplasmáticas (*Desenvolvimento de drogas)
- Indício de inibição da atividade via docking (*Desenvolvimento de drogas)

Pan-genômica é uma área recente da genômica que tem como principal objetivo a comparação genômica entre diferentes linhagens de uma mesma espécie.





Identificar a porção conservada do genoma e os eventos de plasticidade genômica.

Tettelin et al (2005)

UFTM

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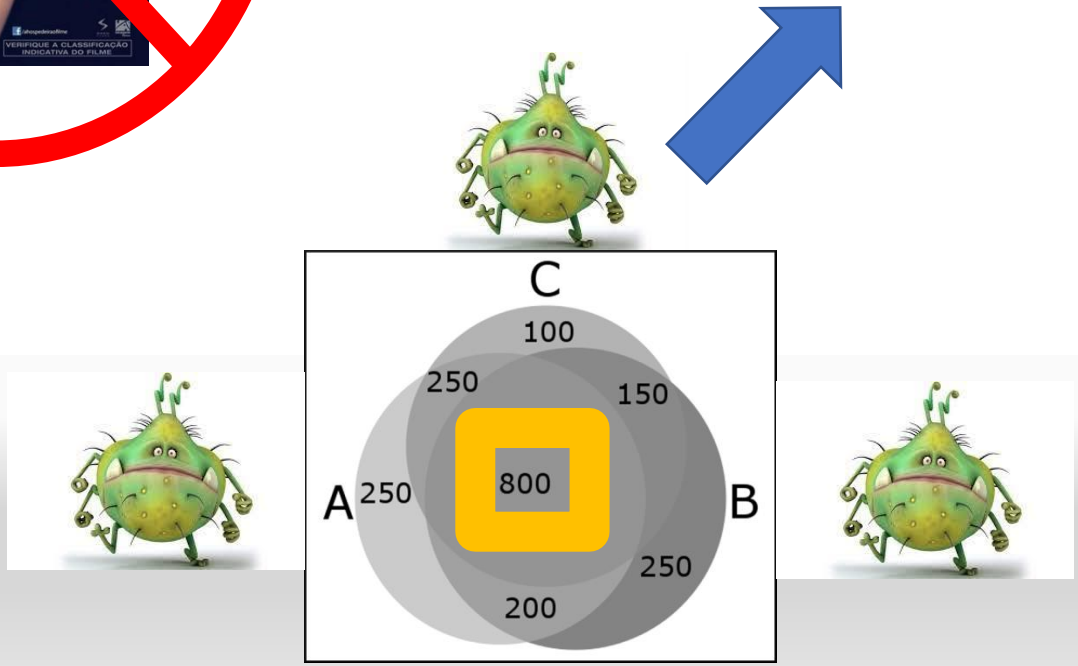

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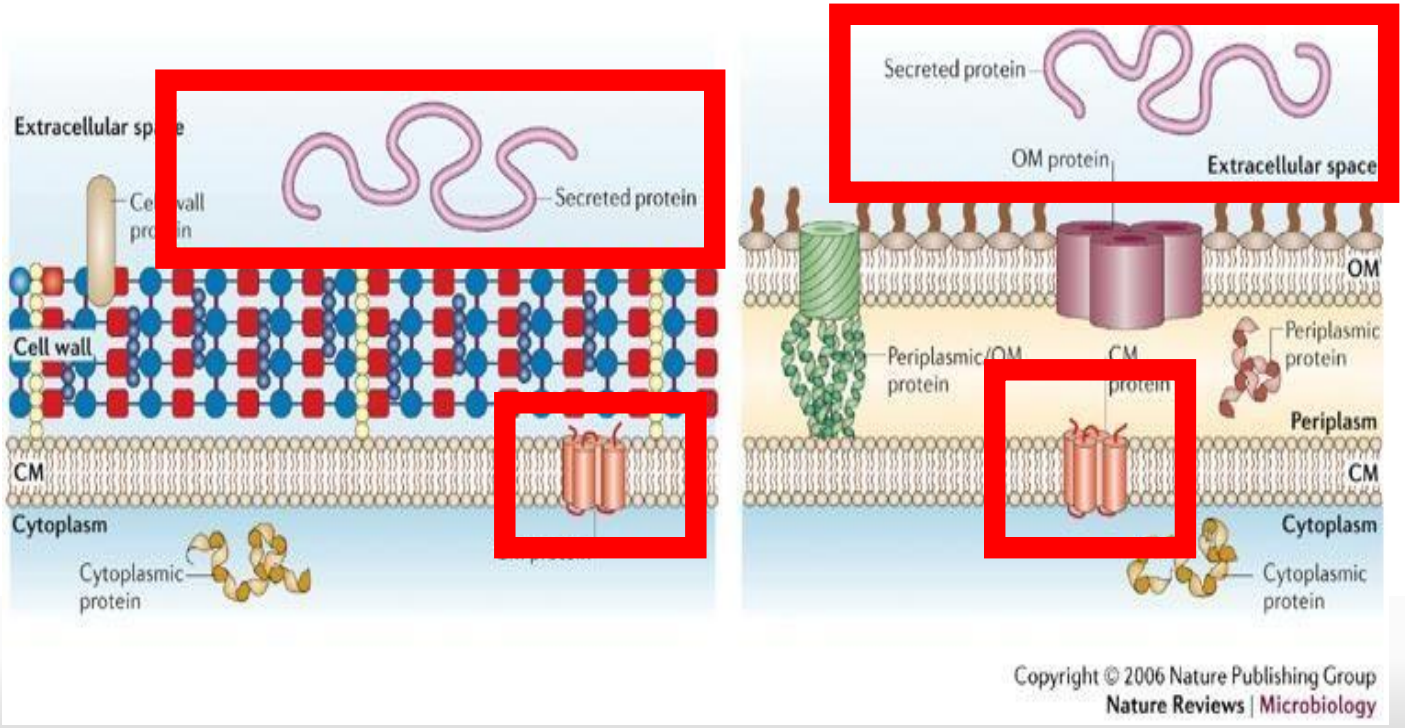

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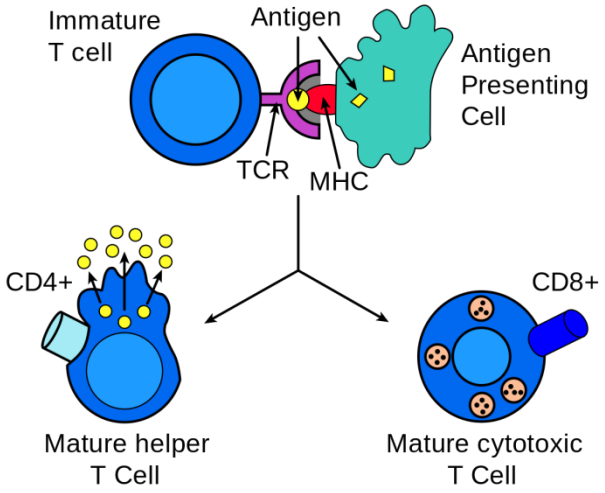

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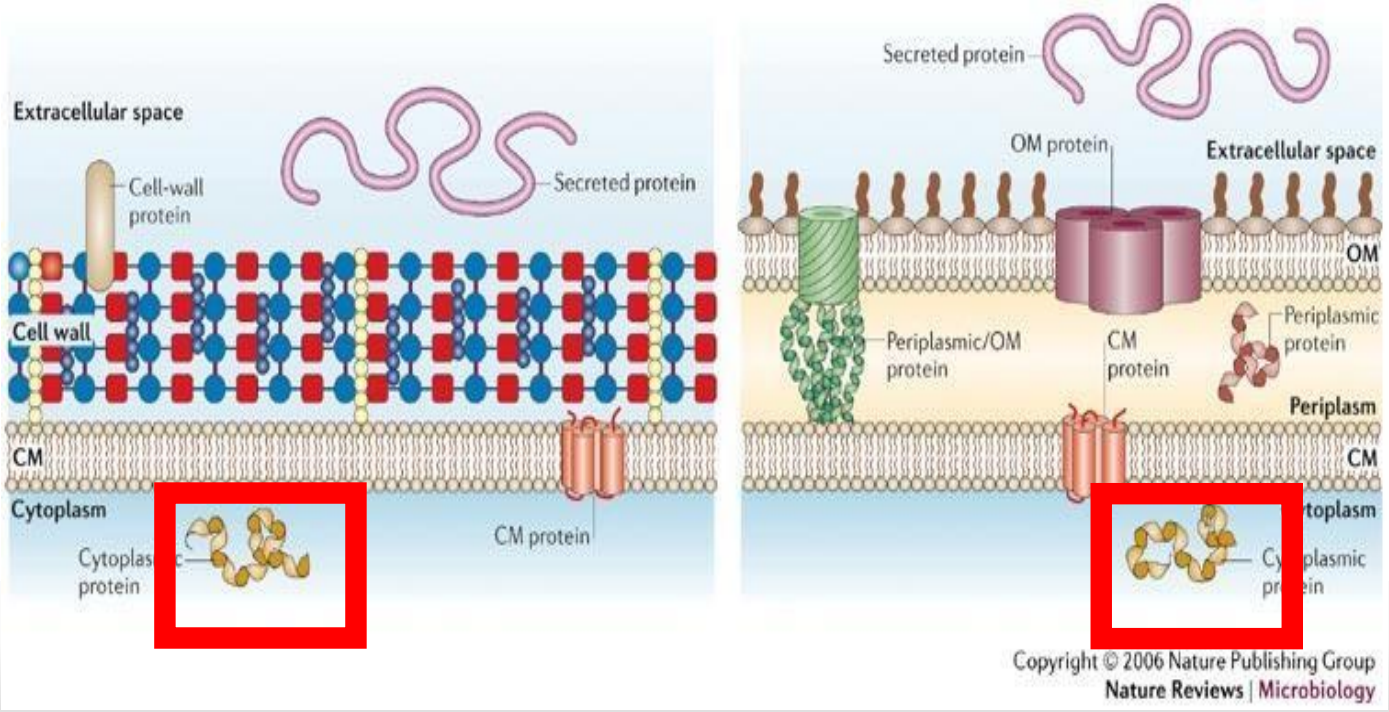

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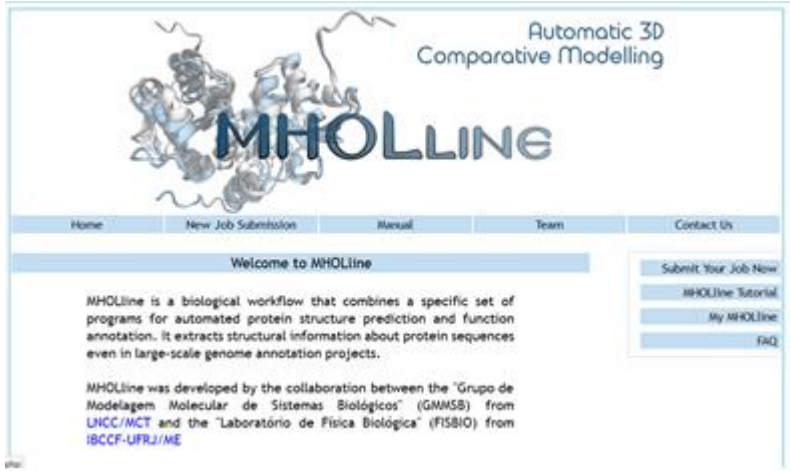

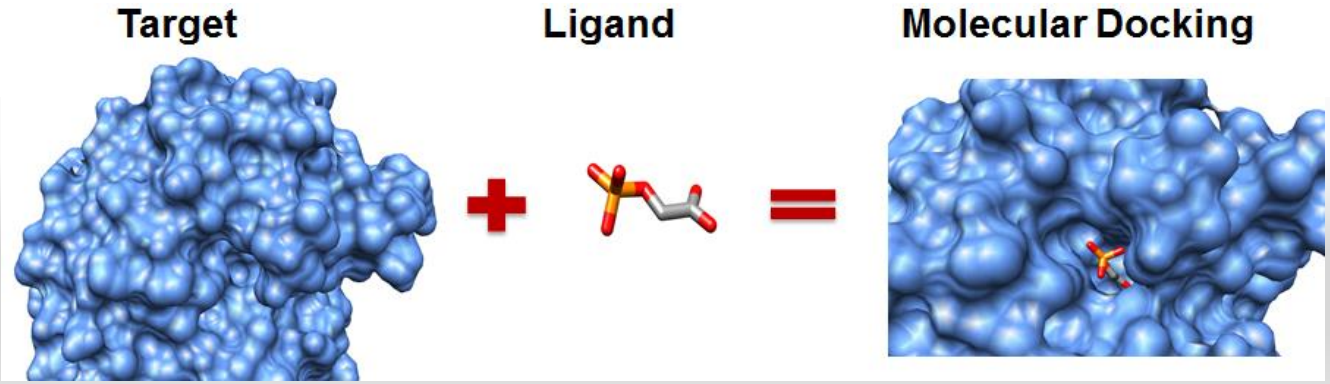

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International Journal of
Molecular Sciences

MDPI

Article

An In Silico Identification of Common Putative Vaccine Candidates against *Treponema pallidum*: A Reverse Vaccinology and Subtractive Genomics Based Approach

Arun Kumar Jaiswal [1,2], Sandeep Tiwari [1], Syed Babar Jamal [1], Debmalya Barh [1,3], Vasco Azevedo [1] and Siomar C. Soares [2,*]

1 Institute of Biological Sciences, Federal University of Minas Gerais, Belo Horizonte 31270-901, MG, Brazil; arunjaiswal1411@gmail.com (A.K.J.); sandip_sbtbi@yahoo.com (S.T.); syedbabar.jamal@gmail.com (S.B.J.); dr.barh@gmail.com (D.B.); vascoariston@gmail.com (V.A.)
2 Department of Immunology, Microbiology and Parasitology, Institute of Biological Sciences and Natural Sciences, Federal University of Triângulo Mineiro (UFTM), Uberaba 38025-180, MG, Brazil
3 Centre for Genomics and Applied Gene Technology, Institute of Integrative Omics and Applied Biotechnology (IIOAB), Nonakuri, Purba Medinipur, West Bengal 721137, India
* Correspondence: siomars@gmail.com

Academic Editor: Christopher Woelk
Received: 14 November 2016; Accepted: 27 January 2017; Published: 14 February 2017

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Research

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Cite this article: Vilela Rodrigues TC *et al.* 2019 Reverse vaccinology and subtractive genomics reveal new therapeutic targets against *Mycoplasma pneumoniae*: a causative agent of pneumonia. *R. Soc. open sci.* **6**: 190907. http://dx.doi.org/10.1098/rsos.190907

Received: 17 May 2019
Accepted: 4 July 2019

Subject Category:

Reverse vaccinology and subtractive genomics reveal new therapeutic targets against *Mycoplasma pneumoniae*: a causative agent of pneumonia

Thaís Cristina Vilela Rodrigues[1,†], Arun Kumar Jaiswal[1,2,†], Alissa de Sarom[1], Letícia de Castro Oliveira[1,2], Carlo José Freire Oliveira[1], Preetam Ghosh[3], Sandeep Tiwari[2], Fábio Malcher Miranda[2], Leandro de Jesus Benevides[4], Vasco Ariston de Carvalho Azevedo[2] and Siomar de Castro Soares[1]

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MCMXVI

F. prausnitzii: a bacterium involved in several diseases

In Crohn's disease:

Fecal flora

Bacteroides
Peptostreptococci
Coprococci
Clostridium
Escherichia coli

Bifidobacterium
Lactobacillus
Faecalibacterium prausnitzii

Swidsinski et al., 2002; Manichanh et al., 2006; Seksik et al., 2006; Sokol et al., 2009

In other intestinal diseases

F. prausnitzii

Irritable bowel syndrome
Rajilic-Stojanovic M. *et al.*, 2011

Colorectal cancer
Balamurugan R. *et al.*, 2008

Ulcerative colitis
McLaughlin SD. *et al.*, 2010

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MCMXVI

Doutorado em Bioinformática

Table 2. Average Nucleotide Identity

Strains	CNCM_I_4546	CNCM_I_4573	CNCM_I_4644	M21-2	SL3-3	A2-165_PacBio	CNCM_I_4543	CNCM_I_4574	HMI-19	CNCM_I_4540	CNCM_I_4542	CNCM_I_4544	KLE1255	AHMP-21	CNCM_I_4541	CNCM_I_4575	L2-6
CNCM_I_4546	100	97,37	95,03	97,33	97,36	86,23	86,76	86,85	86,02	86,47	87,6	86,88	87,44	85,48	86,57	86,81	85,72
CNCM_I_4573	97,37	100	95,02	97,13	97,19	86,79	86,2	85,99	86,66	87,11	86,86	86,88	87,21	86,01	86,24	88,42	84,64
CNCM_I_4644	95,03	95,02	100	95,09	94,99	86,28	85,88	85,81	85,6	85,81	86,44	86,34	86,57	85,6			
M21-2	97,33	97,13	95,09	100	97,36	86,75	86,03	85,9	85,78	86,48	86,8	86,92	87,35	85,5			
SL3-3	97,36	97,19	94,99	97,36	100	86,16	86,47	86,44	86,21	86,03	86,67	86,85	87,05	85,6			
A2-165_PacBio	86,23	86,79	86,28	86,75	86,16	100	98,08	97,99	97,12	85,21	86,11	85,47	86,22	86,1			
CNCM_I_4543	86,76	86,2	85,88	86,03	86,47	98,08	100	99,9	97,08	84,82	85,58	85,42	85,75	85,8			
CNCM_I_4574	86,85	85,99	85,81	85,9	86,44	97,99	99,9	100	97,1	84,77	85,71	85,26	85,63	86			
HMI-19	86,02	86,66	85,6	85,78	86,21	97,12	97,08	97,1	100	86,08	85,56	85,59	85,59	85,9			
CNCM_I_4540	86,47	87,11	85,81	86,48	86,03	85,27	84,82	84,77	86,08	100	97,62	97,57	97,52	85,0			
CNCM_I_4542	87,6	86,86	86,44	86,6	86,67	86,11	85,58	85,71	85,56	97,62	100	98,46	98,1	85,6			
CNCM_I_4544	86,88	86,88	86,34	86,92	86,85	85,47	85,42	85,26	85,59	97,57	98,46	100	98,14	85,6			
KLE1255	87,44	87,21	86,57	87,35	87,05	86,22	85,75	85,63	85,59	97,52	98,1	98,14	100	85,7			
AHMP-21	85,48	86,01	85,61	85,58	85,6	86,1	85,85	86	85,96	85,03	85,62	85,64	85,73	100			
CNCM_I_4541	86,57	86,24	85,91	86,52	86,3	85,25	85,2	85,02	85,47	87,65	88,09	88,05	87,94	85,1			
CNCM_I_4575	86,81	88,42	86,48	86,79	86,33	86,32	85,9	85,85	86,1	85,7	85,97	85,87	86,52	88,3			
L2-6	85,72	84,64	84,87	85,43	85,34	86,09	85,71	85,99	85,93	85,61	86,13	86,03	86,47	86,2			

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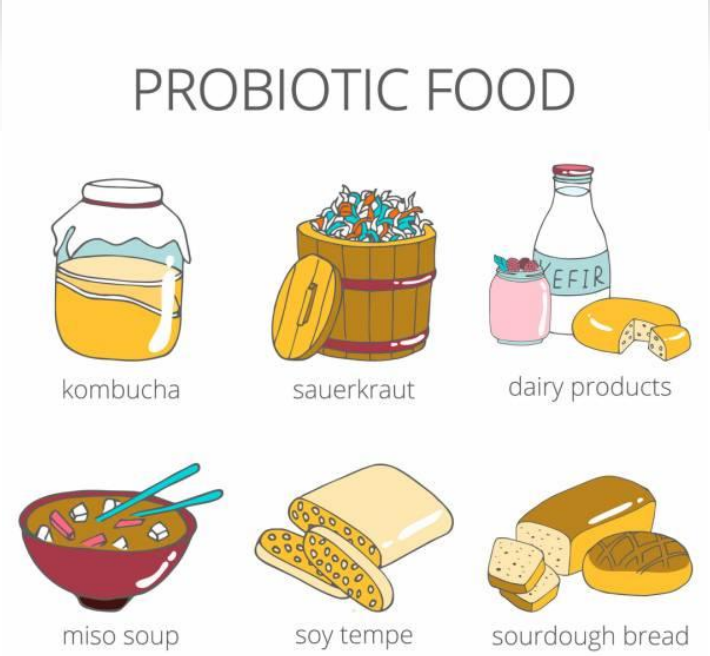

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Locus tag	Gene	Início	Fim	Produto	Localização subcelular
NCDO2118_0139*	*epsK*	144762	145652	Exopolysaccharide biosynthesis protein	Exclusive/ Secreted/ Expressed
NCDO2118_0140*	*epsL*	145677	146600	LytR family transcriptional regulator	Exclusive/ Secreted/ Expressed
NCDO2118_0212*		214606	215988	Hypothetical protein	Exclusive/ Secreted/ Expressed
NCDO2118_0683*		697697	698158	Hypothetical protein	Exclusive/ Secreted/ Expressed
NCDO2118_1420*		1537567	1538422	Hypothetical protein	Exclusive/ Secreted/ Expressed

5 proteínas exclusivas, secretadas e expressas

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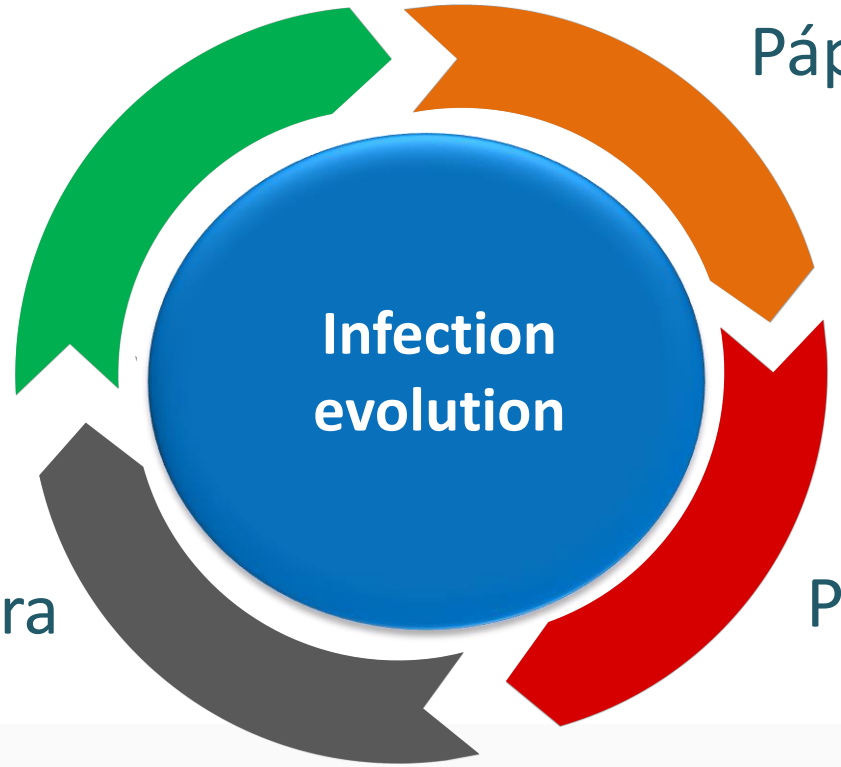

Haemophilus ducreyi

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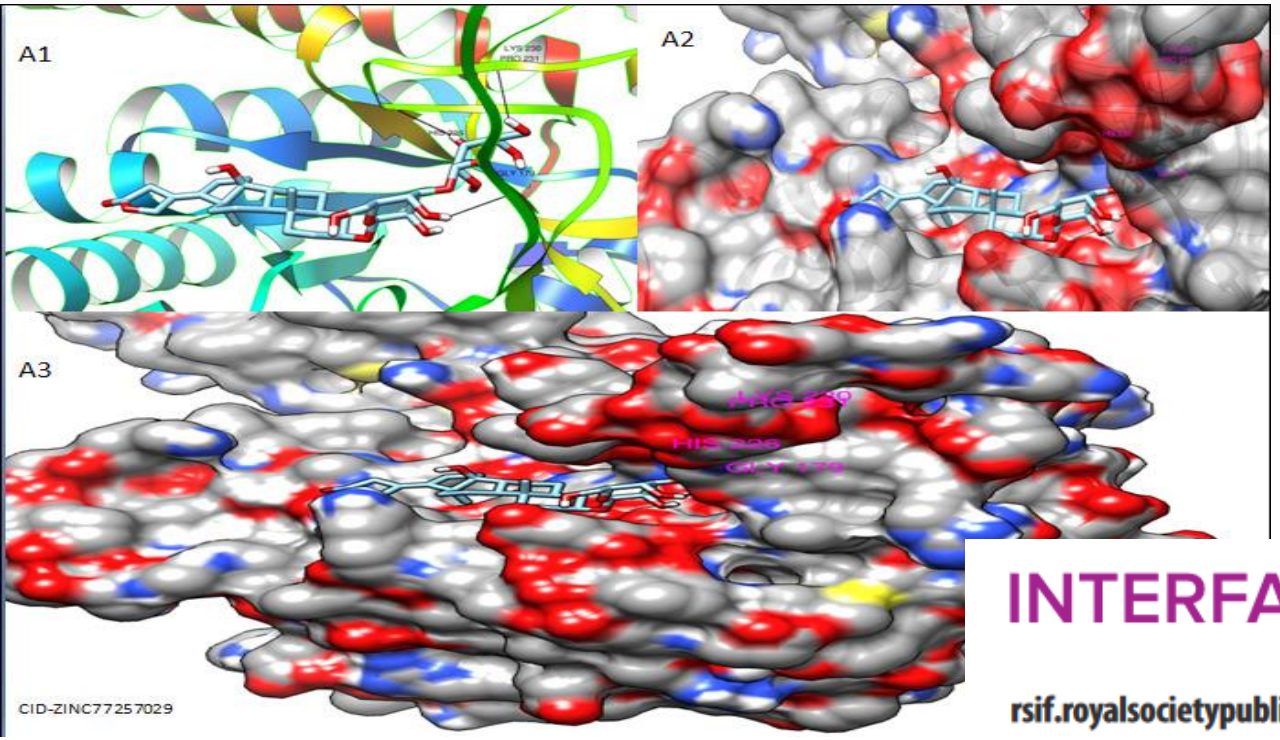

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Alissa de Sarom[1], Arun Kumar Jaiswal[2], Sandeep Tiwari[2], Letícia de Castro Oliveira[2], Debmalya Barh[3], Vasco Azevedo[2], Carlo Jose Oliveira[1] and Siomar de Castro Soares[1,2]

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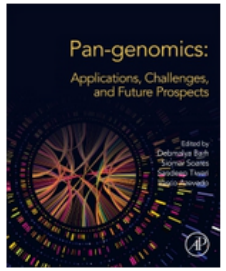

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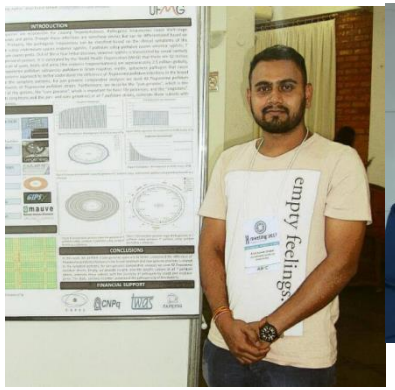

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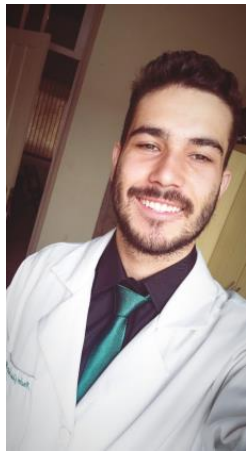

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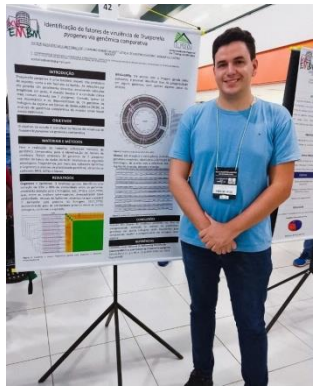

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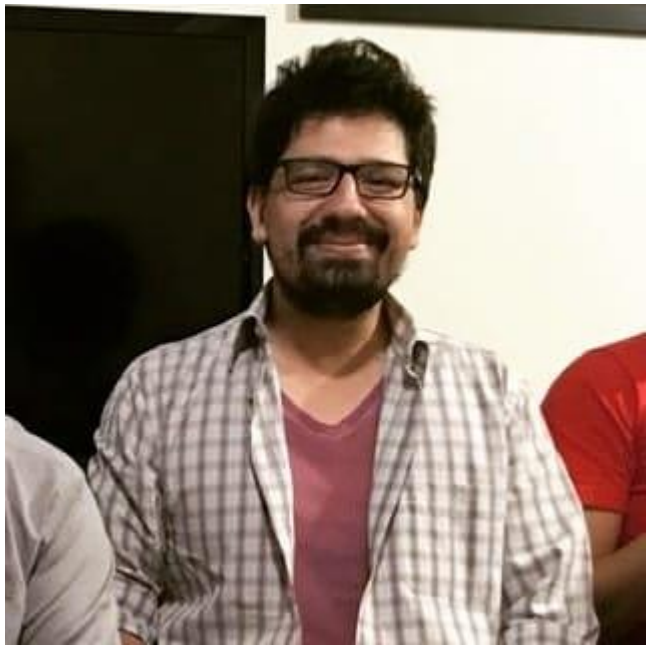
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