

Global Health, Biodiversity, and New Medicine Seminar

“The Quest for natural products with antitrypanosomal and anticancer potential using Computational Biology and Chemistry”

Miguel A. Chávez Fumagalli, PhD



**Universidad Católica
de Santa María**



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Peruvian natural products
database

Peruvian natural products as a source of new pharmacological entities



Table 2. New Chemical Entities and Medical Indication by Source of Compound 01JAN 81–30SEP19^a

indication	total	B	N	NB	ND	S	S/NM	S*	S*/NM	V
Alzheimer's disease	6	1	1		1		3			
COPD	11	2					3		6	
Gaucher's disease	5	3			1				1	
PAH	4						3		1	
Parkinson's disease	14				1	1	6	1	5	
allergic rhinitis	5			1						4
analgesic	19		1		2	11	3	2		
anemia (1 sickle cell)	5	1		1		2			1	
anesthetic	5					5				
antiallergic	18		1	1	4	12				
antianginal	5					5				
antiarrhythmic	17		1			14			2	
antiarthritic	28	8	1	1	4	4	6		4	
antiasthmatic	15	2			3	2	6		2	
antibacterial	162	4	11		78	36			1	32
anticancer	247	52	18	1	43	29	36	13	45	10
anticoagulant	23	5	13				1	1	3	
antidepressant	28				1	8	17		2	
antidiabetic	63	24	1		8	4	16	1	9	
antidote	6	4			1		1			
antiemetic	11					1	2		8	
antiepileptic	20		1		2	11		3	3	
antifungal	34	1			3	27	3			
antiglaucoma	19	1			6	2	6	1	3	
antihistamine	14					14				
antihyperprolactinemia	4				4					
antihypertensive	82		1		2	28	16	2	33	
antiinflammatory	53	1			13	38	1			
antimigraine	13	3				2	1		7	
antinarcolepsy	5				1	2	1		1	
antiobesity	6				1	1	4			
antiparasitic	20		2		7	6		3		2
antipsoriatic	21	12		1	3	1	2	1	1	
antipsychotic	12					4	6		2	

- N= unaltered natural product
- ND= natural product derivative
- S= synthetic drug
- S*= synthetic drug (NP pharmacophore)

“...natural products still hold out the best options for finding novel agents/active templates, which when worked on in conjunction with synthetic chemists and biologists, offer the potential to discover novel structures that can lead to effective agents in a variety of human diseases.” Newman & Cragg 2020.



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Article | [Open access](#) | [Published: 10 May 2023](#)

PeruNPDB: the Peruvian Natural Products Database for in silico drug screening

[Haruna L. Barazorda-Ccahuana](#), [Lena Gálvez Ranilla](#), [Mayron Antonio Candia-Puma](#), [Eymi Gladys Cárcamo-Rodriguez](#), [Angela Emperatriz Centeno-Lopez](#), [Gonzalo Davila-Del-Carpio](#), [José L. Medina-Franco](#) & [Miguel Angel Chávez-Fumagalli](#) 

[Scientific Reports](#) **13**, Article number: 7577 (2023) | [Cite this article](#)

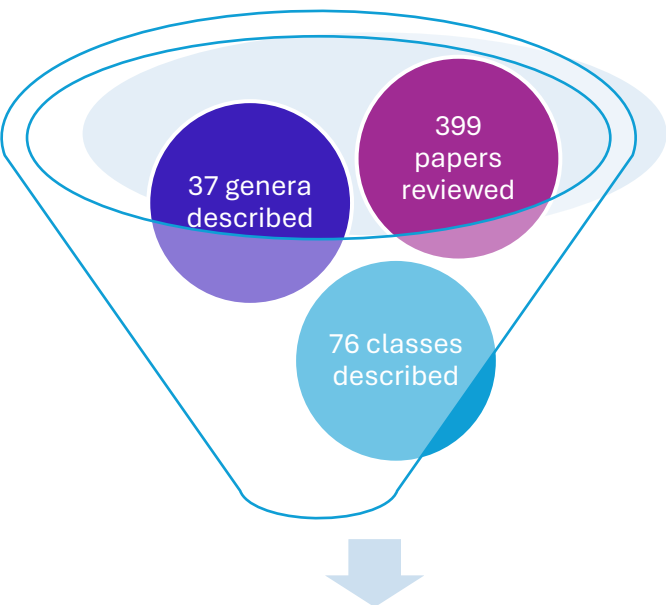
2725 Accesses | **3** Citations | **9** Altmetric | [Metrics](#)



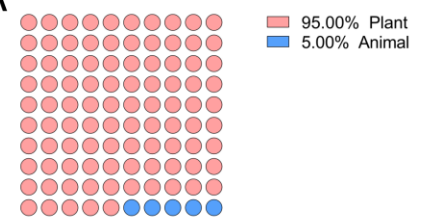


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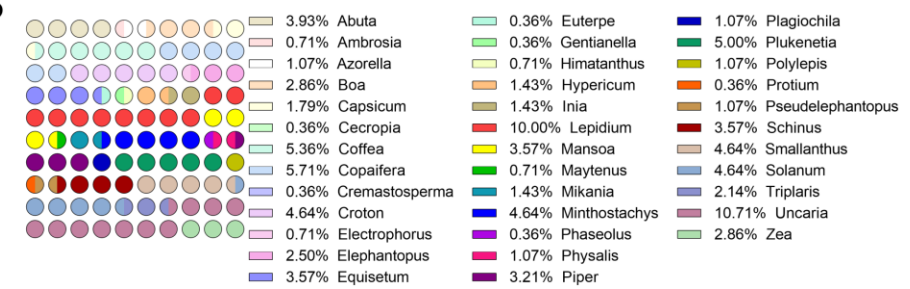
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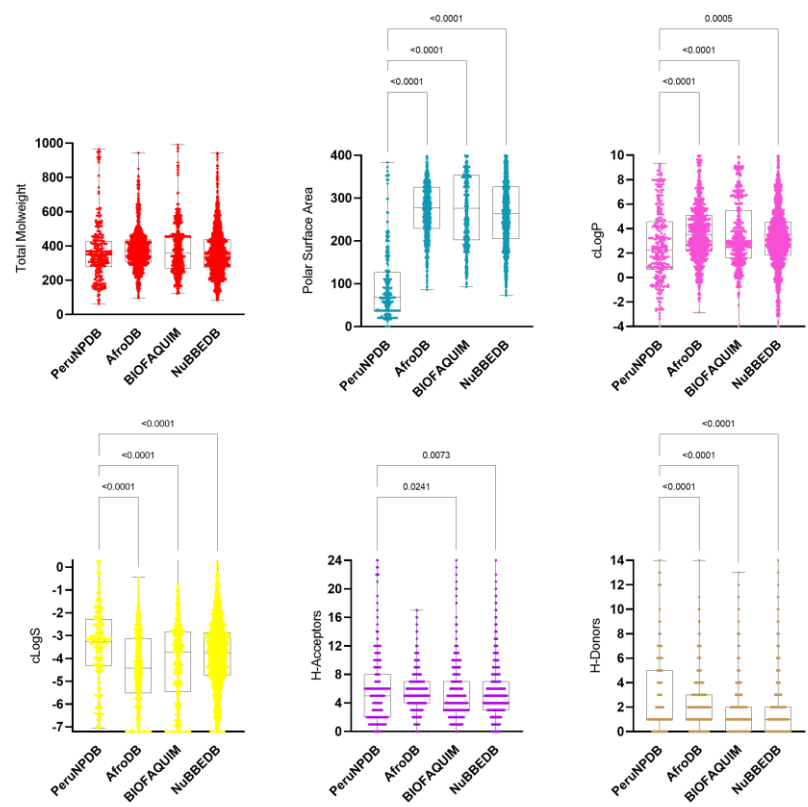
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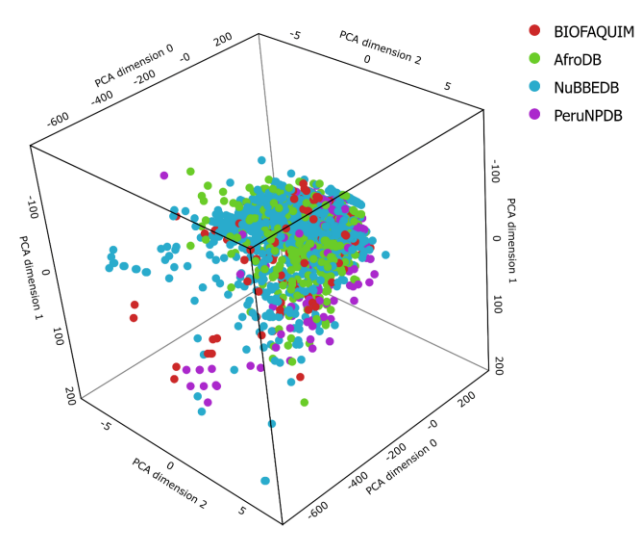


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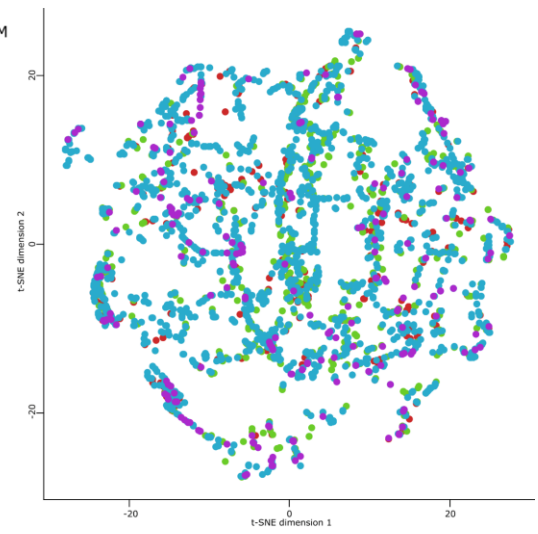
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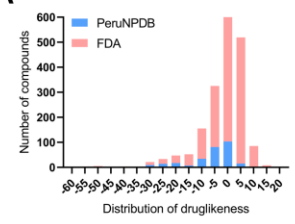
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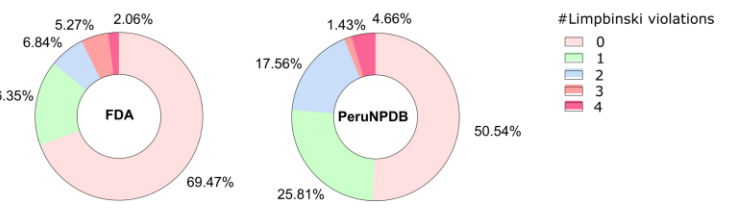
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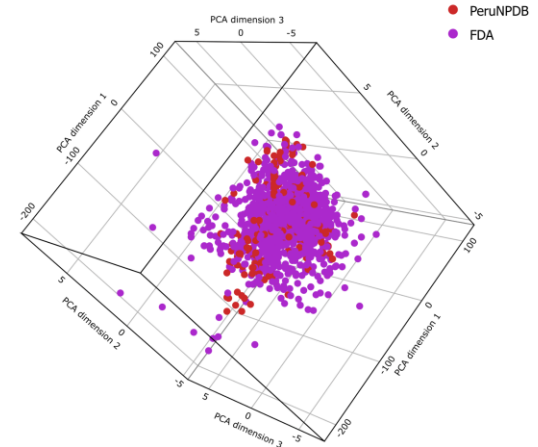
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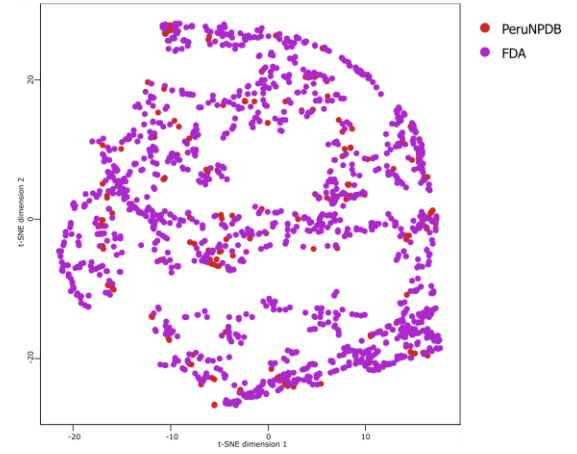
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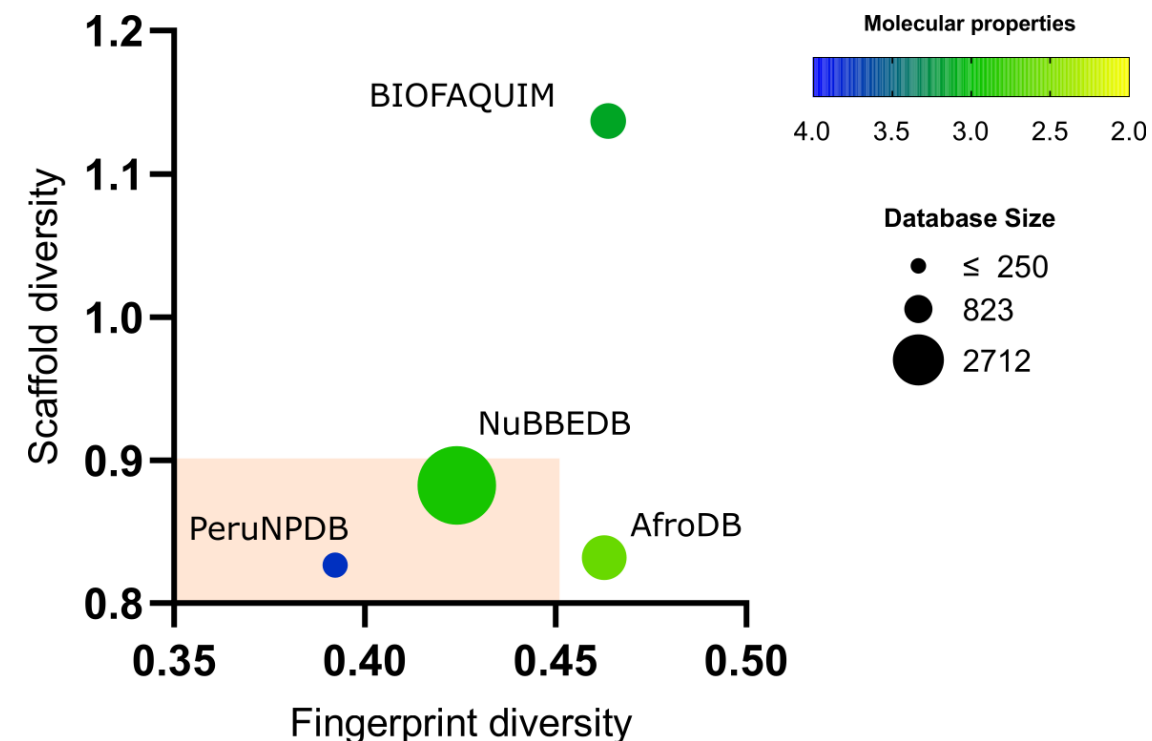
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pharmaceuticals



Article

Navigating the Chemical Space and Chemical Multiverse of a Unified Latin American Natural Product Database: LANaPDB

Alejandro Gómez-García¹, Daniel A. Acuña Jiménez², William J. Zamora^{2,3,4}, Haruna L. Barazorda-Ccahuana⁵, Miguel Á. Chávez-Fumagalli⁵, Marilia Valli⁶, Adriano D. Andricopulo⁶, Vanderlan da S. Bolzani⁷, Dionisio A. Olmedo⁸, Pablo N. Solís⁸, Marvin J. Núñez⁹, Johny R. Rodríguez Pérez^{10,11}, Hoover A. Valencia Sánchez¹⁰, Héctor F. Cortés Hernández¹⁰ and José L. Medina-Franco^{1,*}

Profiling the natural product-likeness of Latin American compound libraries

Alejandro Gómez-García¹, Ann-Kathrin Prinz², Daniel A. Acuña Jiménez³, William J. Zamora^{3,4,5}, Haruna L. Barazorda-Ccahuana⁶, Miguel Á. Chávez-Fumagalli⁶, Marilia Valli⁷, Adriano D. Andricopulo⁷, Vanderlan da S. Bolzani⁸, Dionisio A. Olmedo⁹, Pablo N. Solís⁹, Marvin J. Núñez¹⁰, Johny R. Rodríguez Pérez^{11,12}, Hoover A. Valencia Sánchez¹¹, Héctor F. Cortés Hernández¹¹, Oscar M. Mosquera Martinez¹³, Oliver Koch^{2,*}, José L. Medina-Franco^{1,*}

Fragment Library of Colombian Natural Products: Generation and Comparative Chemoinformatic Analysis

Ana L. Chávez-Hernández¹, Johny R. Rodríguez-Pérez^{2,3}, Hector F. Cortés-Hernández², Hoover A. Valencia-Sanchez², Miguel Á. Chávez-Fumagalli⁴, José L. Medina-Franco^{1,*}



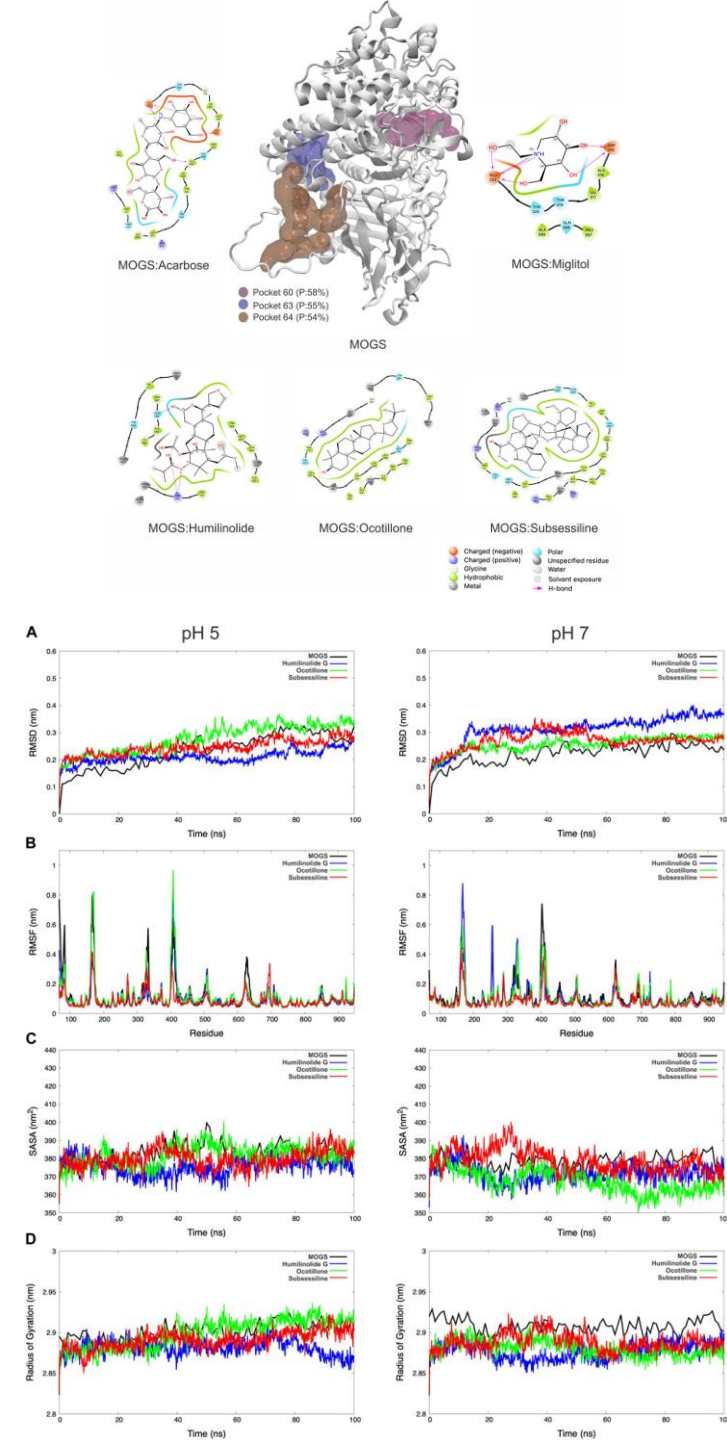
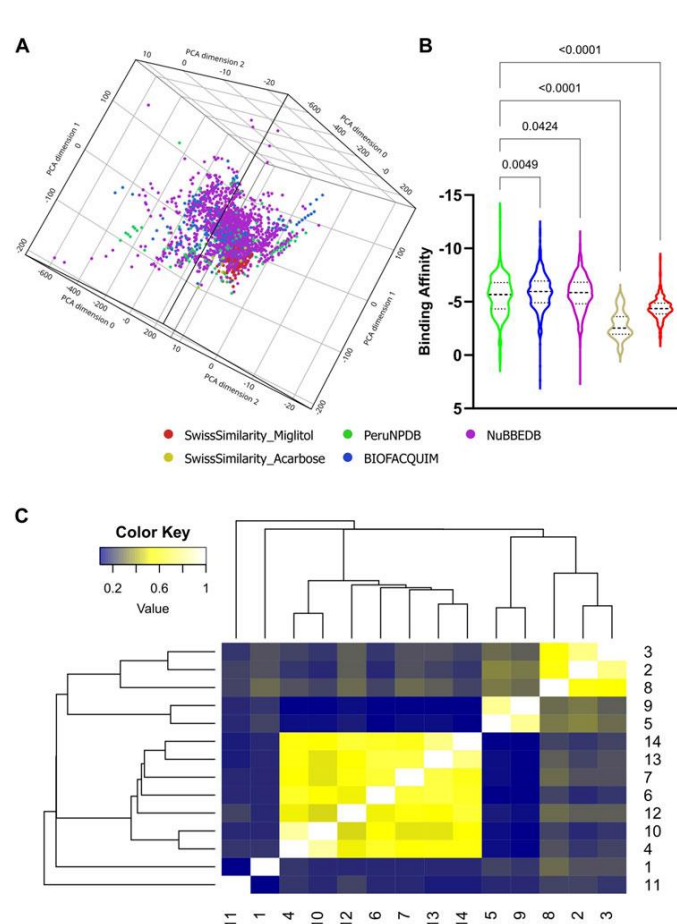
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Targeting *Leishmania infantum* Mannosyl-oligosaccharide glucosidase with natural products: potential pH-dependent inhibition explored through computer-aided drug design

Luis Daniel Goyzueta-Mamani¹,
Haruna Luz Barazorda-Ccahuana¹,
Mayron Antonio Candia-Puma^{1,2}, Alessandro Sobreira Galdino³,
Ricardo Andrez Machado-de-Avila⁴,
Rodolfo Cordeiro Giunchetti^{5,6}, José L. Medina-Franco⁷,
Mónica Florin-Christensen^{8,9},
Eduardo Antonio Ferraz Coelho^{10,11} and
Miguel Angel Chávez-Fumagalli^{1*}





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Article

Antiviral Activity of Metabolites from Peruvian Plants against SARS-CoV-2: An In Silico Approach

by  Luis Daniel Goyzueta-Mamani ^{1,*}  ,  Haruna Luz Barazorda-Ccahuana ^{1,*}  ,
 Karel Mena-Ulecia ^{2,3}   and  Miguel Angel Chávez-Fumagalli ¹  



RESEARCH ARTICLE

Identification of compounds from natural Peruvian sources as potential inhibitors of SARS-CoV-2 Mpro mutations by virtual screening and computational simulations [version 1; peer review: 1 approved with reservations]



Haruna Luz Barazorda-Ccahuana ¹, Eymi Gladys Cárcamo Rodríguez^{1,2},
Angela Emperatriz Centeno-Lopez^{1,2}, Margot Paco-Chipana ¹,
Luis Daniel Goyzueta-Mamani ^{1,3}, Miguel Angel Chavez-Fumagalli ¹

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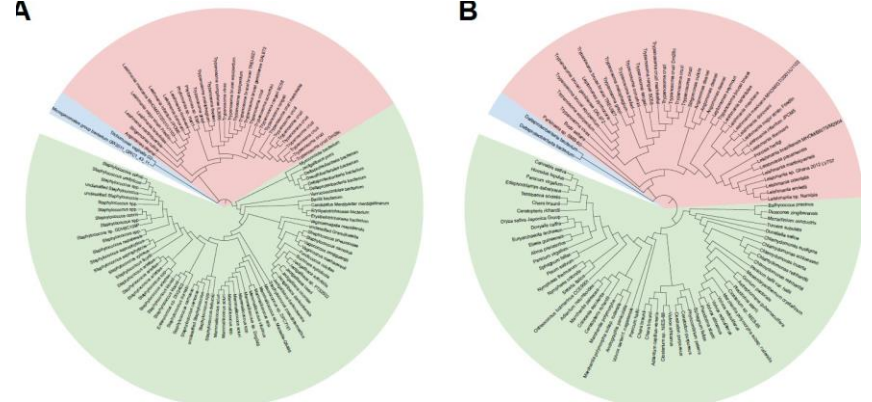
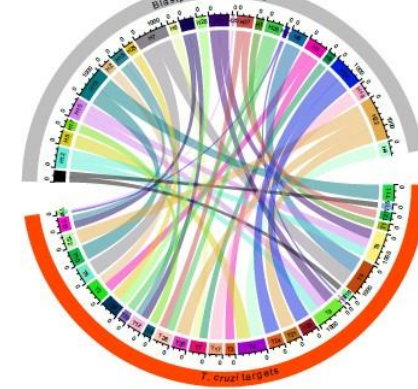
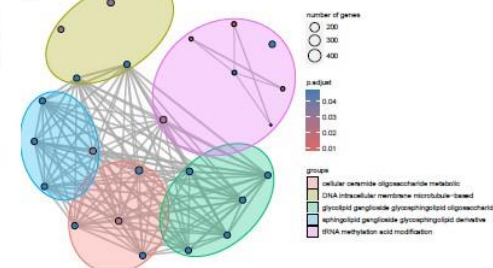
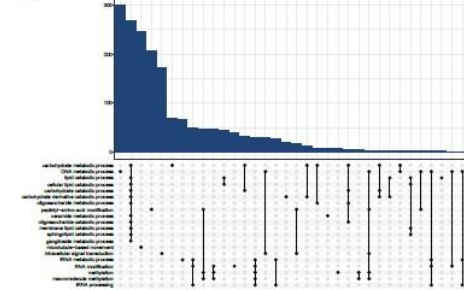
Article

In Silico Analysis of Metabolites from Peruvian Native Plants as Potential Therapeutics against Alzheimer's Disease

by  Luis Daniel Goyzueta-Mamani ^{1,*}  ,  Haruna Luz Barazorda-Ccahuana ²  ,
 Miguel Angel Chávez-Fumagalli ¹  ,  Karla Lucia F. Alvarez ¹  ,
 Jorge Alberto Aguilar-Pineda ¹  ,  Karin Jannet Vera-Lopez ¹   and
 Christian Lacks Lino Cardenas ^{3,*}  



A



- Brazil
- Costa Rica
- El Salvador
- Mexico
- Panama
- Peru



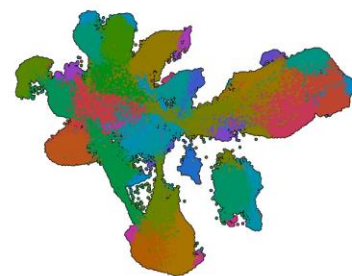
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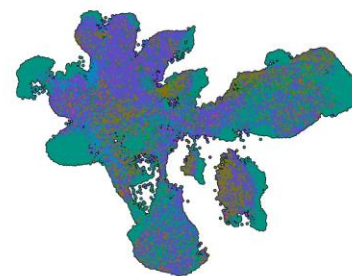


Upcoming Results-HCC

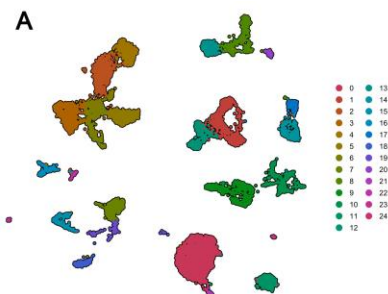
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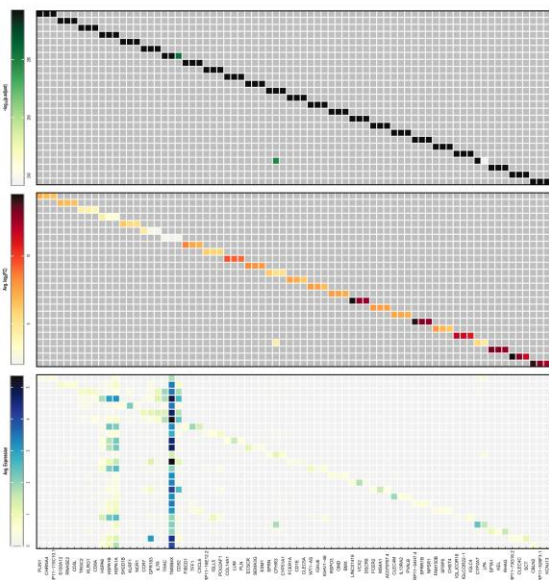


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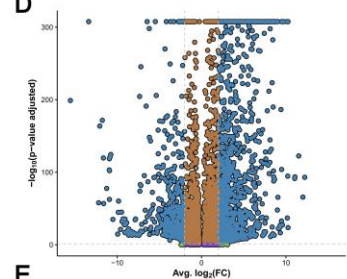


● Disease_Liver
● Healthy_Liver

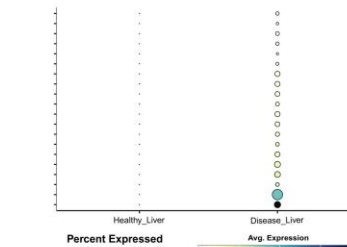
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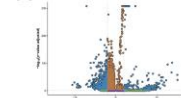
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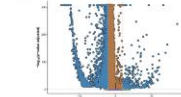
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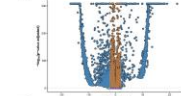
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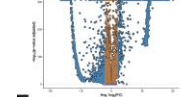
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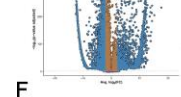
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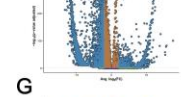
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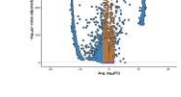
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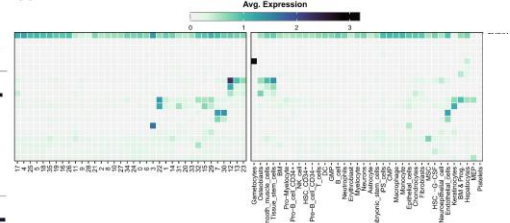
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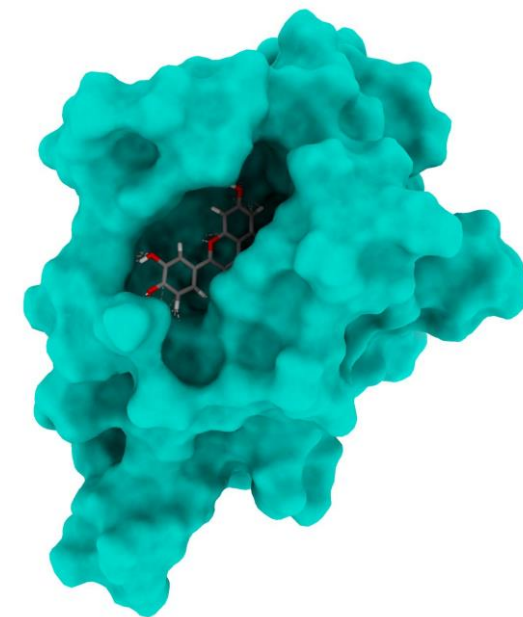
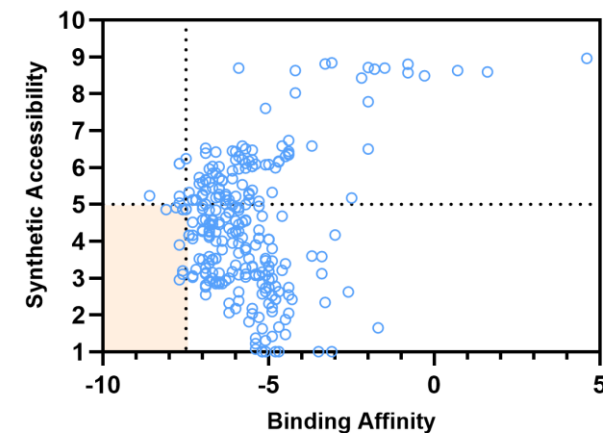
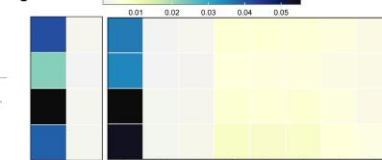
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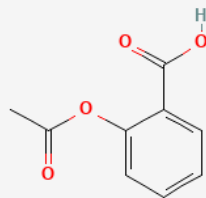


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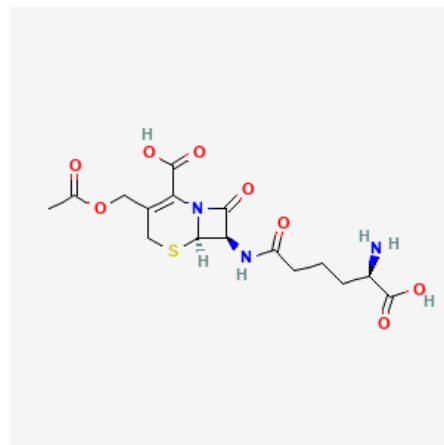
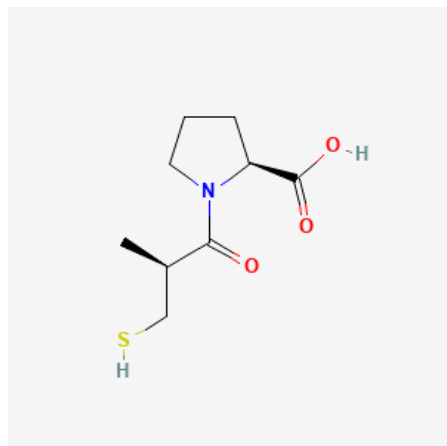
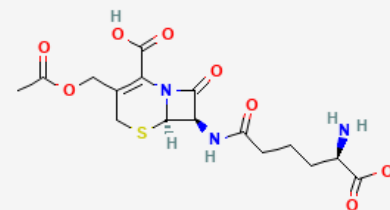
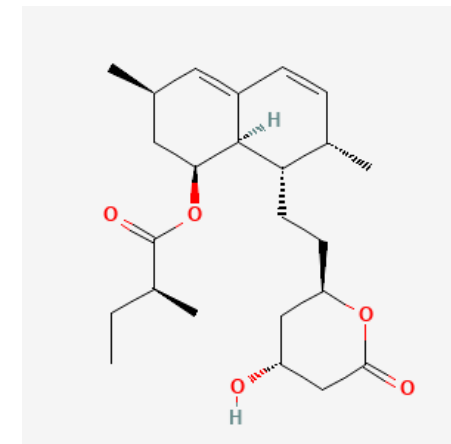
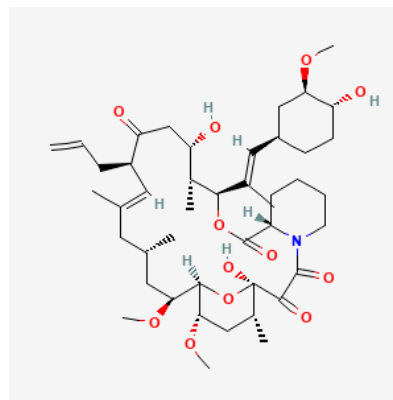
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Upcoming Research



- Antiparasitic
- Antibiotics
- Antifungals
- Antivirals
- Anticancer



- Neurogenerative diseases
- Emerging contaminants
- Theragnostic molecules

Miguel A. Chavez Fumagalli, PhD
mchavezf@ucsm.edu.pe



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