Book of Abstracts

Editors:

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Part 1: About the Workshop

FREE HYBRID WORKSHOP ON SECONDARY METABOLITE DISCOVERY (27th-29th FEBRUARY 2024)

CAiSMD 2024: Computational Applications in Secondary Metabolite Discovery

All the workshop related links are available here:
https://bharatyuva.org/index.php/caismd/workshop2024

What to expect

Over the course of three days, participants in this online workshop will delve into the exploration of modern computer-based approaches for discovering natural products (or secondary metabolites) in the omic age. Esteemed experts will deliver keynote lectures, facilitate hands-on sessions, lead round table discussions, and conduct oral presentations. Early-career scientists and students, who are primarily selected applicants, will have the opportunity to deliver oral presentations lasting between 15 to 30 minutes and present posters in the form of concise flash presentations lasting 5 minutes.

Audience

The workshop is tailored for M.Sc. and Ph.D. students, postdocs, and early-career researchers interested in bioinformatics, chemoinformatics, natural products chemistry, computational drug design, and genomic analysis, particularly within the realm of drug discovery applications.

Registration

To join the workshop, participants are required to fill out the Registration Form
https://bharatyuva.org/index.php/caismd/registration-form-2024.
Those planning to present during the event must submit an abstract using the provided template. All applications for participation must be submitted by the deadline of February 26th, 2024, by midnight CET.

Abstract submission

Abstract submissions for oral presentations (keynotes, standard oral presentations, and flash presentations) must be received by midnight on February 22nd, 2024, CET. The finalized program will be published by February 26th, 2024.

Keynote presentations/Round table discussions

Renowned experts will be directly invited by the organizers to deliver keynote lectures and lead round table discussions, which will typically last between 30 to 60 minutes.

Hands-on session

Selected experts will be invited by the organizers to provide lectures and practical sessions on specific software tools and web servers, with each session lasting 90 minutes.

Oral presentations

Presentations will be allocated up to 15 minutes each and will be selected from applicants who submit an abstract using the provided template by the deadline of February 22nd, 2024, before midnight (CET).

Poster/flash presentations

M.Sc. and Ph.D. students with selected posters will present them in concise 5-minute flash presentations. All submissions must be received by the deadline of February 20th, 2024, before midnight CET. Presentations not accepted as standard (15 minutes) oral presentations will be automatically assigned as flash presentations or may be rejected. Poster stands are a limited number, so only selected posters will be presented.

Time zone

All workshop events follow Central European/West African Time.

Lecture option and web platform

Presenters are required to upload their lecture slides 24 hours before the workshop, which will then be available for download by workshop participants.

Certificate of participation

Attendees who participate in at least 60% of all lectures and complete an online post-workshop survey will receive a signed certificate of participation.

Cost of participation

Participation in the online workshop is free of charge. However, there will be a fee for onsite/in-person attendance, which is 5,000 FCF cash. Mobile money payment is also acceptable with the required fees. Kindly contact these numbers to make arrangements for in person participants before arrival in Buea or to the workshop venue. Tel: 670935132 (MTN) and 691280058 (Orange). Name: Ariane Tirr Ndi.

Language of workshop

The workshop will be conducted in English.

Workshop materials

Attendees will have access to a book of abstracts, lecture slides, hands-on tutorials, and a YouTube channel containing videos of lectures.

Deadlines

- Registration last date

Deadline Date: 26-Feb-2024 Task: Register on this link

- Submission of Abstracts

Deadline: 22-Feb-2024 Task: Submit abstracts for keynotes, oral presentations, and hands-on sessions here

- Poster Presentation Abstract Submission

Deadline Date: 20-Feb-2024 Task: Submit abstracts for poster presentations (only applicable for in-person attendance) here

Workshop link

CAiSMD 2024 will run on the same link for all three days (February 27, 2024 – February 29, 2024) · Time zone: CET on Google Meet

Video call link:

https://meet.google.com/eib-uyyb-wi

Part II: Workshop Programme

HS = Hands-on Session. KL = Keynote Lecture, OP = Oral Presentation, RTD = Round Table Discussion, YI = Young Investigator Session

Day 1: 27 February 2024

Time	**Event (Chair: Jutta Ludwig-Müller)**
01:45 pm	Opening of the Workshop
02:00 pm	*KL01* (Samuel Egieyeh, 45 min)
02:45 pm	Break
03:00 pm	*HS01* and *HS02* Parallel Hands-on Sessions (Yannick Djoumbou-Feunang and Janez Konc, 90 min)
04:30 pm	Announcements and End of Day 1

Day 2: 28 February 2024

Time	**Event (Chair: Fidele Ntie-Kang)**
09:00 am	*OP01* (Marko Jukic, 20 min)
09:20 am	*OP02* (Gemma Turon, 20 min)
09:40 am	*OP03* (Joel O. Onoja, 20 min)
10:00 am	*OP04* (Paul Zierep, 20 min)

10:20 am: Coffee break (15 min)

Time	**Event (Chair: Fidele Ntie-Kang / Daniel M. Shadrack)**
10:35 am	*RTD01* (All lecturers of day 1 and first part of day 2, 45 min)
11:20 am	*OP05* (Padmika Wadanambi, 20 min)
11:40 am	*OP06* (Boris D. Bekono, 20 min)

12:00 pm: Lunch break (120 min)

Time	**Event (Chair: Samuel Egieyeh)**
02:00 pm	*KL02* (Vanderlan da Silva Bolzani, 45 min)

02:45 pm: Coffee break (15 min)

Time	**Event (Chair: Samuel Egieyeh)**
03:00 pm	*HS03* and *HS04* Parallel Hands-on Sessions (Paul Zierep, Daniel M. Shadrack, Thommas M. Musyoka and Fidele Ntie-Kang, 90 min)
04:30 pm	Announcements and Closing of Day 2

Day 3: 29 February 2024

Time	Event (Chair: Fidele Ntie-Kang/Donatus B. Eni)
08:00 am	*TY* (Test yourself exercises from the parallel HS, 60 min)
09:00 am	*KL03* (Andres Vasquez, 45 min)

09:45 am: Coffee break (15 min)

Young Investigators Session (from selected submitted abstracts or MSc, PhD students and emerging postdoctoral researchers)

Time	Event (Chair: James A. Mbah / Paul Zierep / Jonathan A. Metuge)
10:00 am	*YI01* (Hannah Augustijn, 15 min)
10:15 am	*YI02* (Evgenii Ziaikin, 15 min)
10:30 am	*YI03* (Kojom Foko, 15 min)
10:45 am	*YI04* (Wilberforce Ndarawit, 15 min)
11:00 am	*YI05* (Donatus B. Eni, 15 min)
11:15 am	*YI06* (Bruno D. A. Akamba, 15 min)
11:30 am	*YI07* (Kamche Aubin Youbi, 15 min)
11:45 am	*YI08* (Martial Judicael Peyieno, 15 min)
12:00 noon	*YI09* (Jude Y. Betow, 15 min)
12:15 pm	*YI10* (David Kitheka, 15 min)
12:30 pm	*YI11* (Samphelix O. Obende, 15 min)
12:45 pm	*YI12* (Daniel Moscoh Ayine-Tora, 15 min)

01:00 pm**: Lunch break (30 min)**

Time	Event (Chair: Fidele Ntie-Kang/Donatus B. Eni)
01:30 pm	*RTD02* (Jose L. Medina-Franco, 30 min)
02:00 pm	Closing remarks

Hands-on Sessions

Day 1: *HS01* Yannick-Djoumbou-Feunang (Bioinformatics)

Day 1: *HS02* Janez Konc (Chemoinformatics)

Day 2: *HS03* Paul Zierep (Bioinformatics)

Day 2: *HS04* Daniel M. Shadrack / Thommas M. Musyoka / Fidele Ntie-Kang (Chemoinformatics)

Part III: Abstracts

KL01: Computational studies on selected phytochemical constituents of some antimalarial plants identified potential inhibitors of wildtype and mutant forms of dihydrofolate reductase-thymidylate synthase

Moses Ikegbunam[1,2], Mary Ejiofor Innocent[3] Valentine Onwuakpa[1], Amarachi Akachukwu[4], Emmanual Oranu[5], Jude Okoyeh[6] and * Samuel Egieyeh[7]

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Resistance to pyrimethamine, an antimalarial medicine, has been reported due to mutations in its target, the Dihydrofolate reductase-thymidylate synthase (DHFR-TS). Phytochemicals have been reported to have privileged structures that might bind strongly to multiple targets or mutants of the same targets [1]. This study aims to identify phytochemicals of *Acalypha wilkesiana, Cymbopogon citratus, Azadirachta indica*, and *Morinda lucida* with high binding affinities for the wildtype and mutants of *Plasmodium falciparum* DHFR-TS. The 3D structures of the selected phytochemicals were obtained from PubChem while the protein model of the wildtype and mutant forms of DHTR-TS were downloaded from Protein Databank (PDB). All chemical structures and models were appropriately prepared for molecular docking simulations. High throughput virtual screening was implemented, after the validation of docking protocols, with AutoDock-Vina 1.1.2. Phytochemicals with better binding affinities to the wildtype and three mutants of DHTR-TS than pyrimethamine were selected for high-precision molecular docking with Schrodinger Maestro and molecular dynamics simulation on Galaxy EU (https://galaxyproject.eu/.). Four phytochemicals showed higher binding affinities to the wildtype and mutant forms of DHFR-TS than pyrimethamine. Molecular dynamics of the complex of top binding phytochemical (rosmarinic acid) to the double mutant revealed lower free binding energy (KJ/mol) during the simulation in comparison to the pyrimethamine and mutant complex. In congruence, the Root Mean Square Deviation (RMSD) plot revealed that the rosmarinic acid-double mutant complex was more stable than the pyrimethamine-double mutant complex. Molecular docking predicted four phytochemicals with higher binding affinities to the wild-type and mutant forms of DHFR-TS. Molecular dynamics showed higher strength of interaction and greater stability of the interaction of one of the phytochemicals to the double mutant form of DHFR-TS. Further studies will be carried out in-vitro and in-vivo to validate the results of this study.

Keywords: Malaria, Resistance, Mutation, Virtual screening, Dihydrofolate Reductase–Tymidylate Synthase

KL02: Natural products from Brazilian biodiversity, small or large always remarkable

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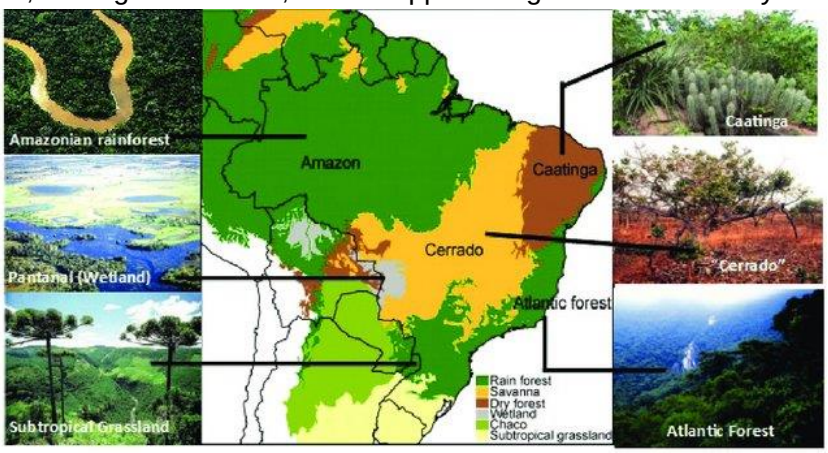
The plant chemical diversity is fantastic, and natural product molecular structures are reflected in a large variety of biochemical reaction pathways, which are responsible for several classes of biologically active secondary metabolites. This metabolic complexity is fundamental for the communication, regulation, and defense of the species, in the most diverse ecosystems and, particularly in extreme habitats, due to the fantastic chemical diversity of small and large molecules biosynthesized by plants, and other organisms of the terrestrial biodiversity. In Brazil we are facing several biomes and the Cerrado - an extremely environment, the second largest after the Amazon, due to its characteristics, unique in the world, has a special vegetation for looking for natural products, which still chemically and pharmacologically understudied, as, peptides and polysaccharides. These macromolecules are accumulated in several plant species of this extreme environment and only a very few studies have been carried out with these plants, being therefore, a rich natural laboratory to be chemically and pharmacologically explored. It is also known that the metabolomic study of all primary and secondary metabolites (high and low molecular weight) is being indispensable for mapping all metabolites produced by a species, essential to understanding its survival in terrestrial and aquatic environments. Also, plants small or large metabolites are important supplies to produce drugs, foods, cosmetics, fragrances, colorants, and agrochemicals, which support a vigorous bioeconomy in several countries.



Keywords: Bioproducts, Brazilian Biodiversity, Natural Products, New Trends

References:

[1] Silvério, M.R.S. et al. *Molecules*, **2020**, 25, 3484.
[2] Pang, Z. et al. *Nucleic Acids Research*, **2021**, 49, W388–W396.
[3] Wang, M. et al. *Nature Biotechnology*, **2016**, *34*, 828.

KL03: Greening drug discovery innovation: unleashing the full potential of virtual screening and molecular fragmentation with natural products

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The discovery of pharmacological agents is a complex and costly process that demands the integration of multiple fields. Virtual Screening (VS), as a transformative methodology since its inception in the late 80s, has conventionally expedited the identification of potent compounds, offering the unprecedented advantage of rapidly screening compounds in the order of billions—a landmark typically beyond the reach of conventional high-throughput screening methods. Moreover, VS allows the exploration of molecules not yet synthesized, further expanding the scope of potential drug candidates. However, despite these advancements, the importance of chemical diversity—a criterion deemed crucial by researchers in the last decade—is frequently underestimated, presenting a challenge to the success of drug discovery campaigns. Fragment-based ligand design (FBLD) emerges as a strategic solution in this context, recombining and evolving fragments into ideal drug-sized candidates capable of establishing optimal binding interactions with molecular targets and exhibiting desirable pharmacological properties. Nevertheless, FBLD encounters substantial challenges when the input library lacks sufficient chemical diversity. Natural Products (NPs), despite their inherent complexity, provide a valuable avenue to address these challenges. When strategically combined with FBLD and VS, NPs can significantly enhance the success rates of drug discovery campaigns, offering a unique balance between serving as a rich source of chemical diversity and providing opportunities to explore large, complex molecular entities. The talk will not only elucidate these concepts but also showcase relevant findings applying these technologies, each focused on designing and discovering new agents with inhibitory capacity against diseases such as Cancer, Dengue, Zika, and SARS-CoV-2. Through detailed discussions, we will delve into the methodological strategies employed in each case, along with the associated implications, challenges, and future perspectives tied to the pursuit of innovative molecules with promising therapeutic potential.

OP01: Essential molecular docking steps and identification of binding sites using CmDock

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Molecular docking is a relatively fast *in silico* technique used in structural biology and drug discovery to predict the preferred orientation of a molecule (small molecule or macromolecule; ligand) when bound to target molecule (named receptor). By simulating the interaction between interacting partners, docking algorithms aim to predict the most favorable binding poses as assessed by the scoring function. Results can thus help in understanding molecular recognition and designing new drugs. This method plays a crucial role in virtual screening of potential drug candidates, optimizing their efficacy and minimizing experimental costs. CmDock is an open-source docking software designed for docking ligands against proteins and nucleic acids, with optimizations, quality-of-life improvements, and parallel processing capabilities. Software can conduct high-throughput virtual screening (HTVS) campaigns and anticipate binding modes. Furthermore, quick assessments of binding site locations on the protein can be conducted using whole-protein grid calculations and complete surface search using a set of molecular probes.

Keywords: binding site; docking algorithms; molecular docking; virtual screening

OP02: Open-source AI/ML for antimicrobial drug discovery

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Artificial intelligence (AI)- and machine learning (ML)-based tools have the potential to revolutionize drug discovery, particularly in resource-limited settings, such as infectious and tropical neglected diseases. Ersilia has developed a set of AI/ML-based tools to support medicinal chemistry, parasitology and ADME experimental pipelines, including quantitative structure-activity/property relationship (QSAR/QSPR) modelling (ZairaChem) and de novo molecular generation (ChemSampler). Moreover, we offer our tools via a unified, open-source platform, the Ersilia Model Hub. In this talk, we will present our computational methods and infrastructure and their application to the discovery of new treatments for infectious diseases, exemplifying an end-to-end implementation at the H3D Centre (South Africa) of a virtual screening cascade for malaria and tuberculosis drug discovery that includes key decision-making assays ranging from whole-cell phenotypic screening and cytotoxicity to aqueous solubility, permeability, microsomal metabolic stability, cytochrome inhibition, and cardiotoxicity [1].

Keywords: Artificial Intelligence; Machine Learning; autoML; QSAR

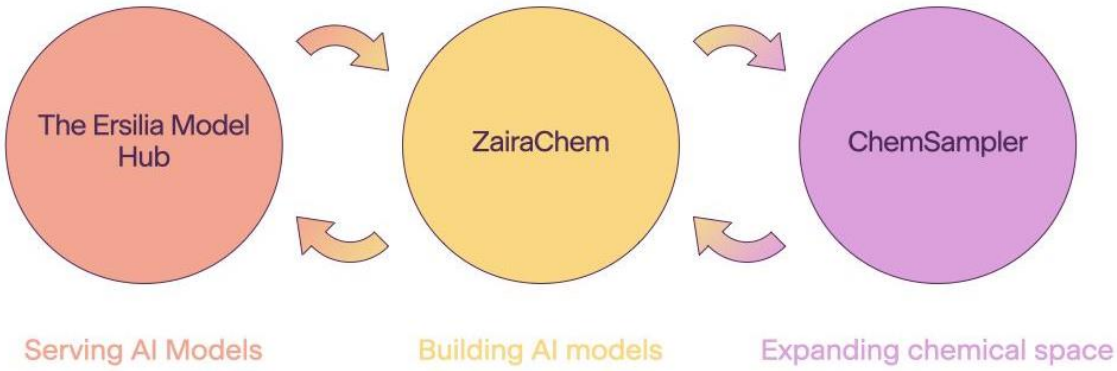

Figure 1: Ersilia's open source toolbox for drug discovery

References:

[1] Turon, G., Hlozek, J., Woodland, J.G. et al. First fully-automated AI/ML virtual screening cascade implemented at a drug discovery centre in Africa. Nat Commun 14, 5736 (2023). https://doi.org/10.1038/s41467-023-41512-2

OP03: A ceramide isolated from *Tinospora cordifolia* (Menispermaceae) with acetylcholinesterase inhibitory activity and molecular docking study

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[4]Department of Biochemistry and Molecular Biology, Faculty of Sciences, Obafemi Awolowo University Ile-Ife, Nigeria.
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Background: Alzheimer's Disease (AD) is a neurological disorder caused by acetylcholinesterase (AChE) via termination of the action of acetylcholine by catalytic hydrolysis. Inhibition of AChE is considered a useful approach to combat AD [1,2]. The study aims to evaluate the AChE inhibitory activity of a compound isolated from the stem of *Tinospora cordifolia*.

Methods: Chromatographic techniques were used to isolate and purify bioactive compounds. Their structures were determined by spectroscopic analysis including 1D and 2D NMR, ^{13}C-NMR, EI-MS, UV, FT-IR. Ellman colorimetric assay method was used to determine the AChE inhibitory activity *in vitro*. The selected PDB was modeled with MOE 2019 using PDB ID: 4EY7 (Human Acetylcholinesterase).

Results: Chromatographic separation yielded one compound. Based on spectroscopic data, the molecule was identified as rel-(2S, 3S, 4R, 1 6E)- 2-[(2'R)-2'-hydroxynonadecanoylamino]-heneicosadec-16-ene-1,3,4-triol reported for the first time in Menispermaceae. The molecule demonstrated good AChE inhibitory activity (IC_{50} = 0.055±0.00 mg/mL) at 0.1 mg/mL compared to eserine (IC_{50} = 0.009±0.00 mg/mL). The docked pose had an abundance of hydrophobic, hydrogen and Pi stacking interaction with the estimated free energy of binding (ΔG), kcal/mol to be (-11.1739).

Conclusion: The ceramide could be a potential lead compound for new acetylcholinesterase inhibitor (AChEi) drug for the management of AD.

Keywords: Acetylcholinesterase inhibition; Ceramide; Menispermaceae; Molecular docking; *Tinospora cordifolia*

References:

[1] Sharma K. Cholinesterase inhibitors as Alzheimer's therapeutics. Molecular Medicine Reports, 20(2), 2019:1479-87.
[2] H Ferreira-Vieira T, M Guimaraes I, R Silva F, M Ribeiro F. Alzheimer's disease: targeting the cholinergic system. Current Neuropharmacology, 14(1), 2016:101-15.

OP04: Investigating secondary metabolite discovery from isolates to metagenomes using Galaxy

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Galaxy [1], is a comprehensive data science and workflow management platform that offers a web-based, intuitive, and user-friendly interface to command-line tools. It automates computation and data provenance management while transparently scheduling workflows, making it easier for scientists to perform complex bioinformatic tasks. Users without access to computing facilities can perform their analysis on public Galaxy instances, such as Galaxy Europe [2], that allow running tools that require large computational resources for everyone. Various tools exist for common tasks in metabolite discovery, such as antiSMASH [3] as well as complete tool libraries for statistics, machine learning [4] and cheminformatics [5]. In recent years, the metagenome tool stack of Galaxy has grown to more than 200 tools [6], providing the possibility to combine metabolite discovery and metagenome analysis workflows, to gain an improved understanding of community dynamics. Galaxy is also connected to large data sources, such as the MGnify database [7], that provides access to metagenome data that was analyzed by standardized workflows and includes taxonomic classification as well as gene cluster predictions. To further extend these analysis capabilities, the Freiburg Galaxy Team is currently working on the integration of dedicated tools, such as BIG-SCAPE [8] and BIG-MAP [9], that allow for gene clusters analysis on metagenomic scale. Here, we would like to present the current capability of Galaxy for secondary metabolite discovery; introduce the microbial community; explain how researchers can get involved; and the envisioned developments. The hands-on session guides users through the basics of Galaxy and introduces some examples, that can be used as a starting point to develop complex secondary metabolite discovery and joint metagenome analysis workflows. The participants can follow the hands-on session on the public Galaxy Europe instance.

Keywords: Secondary Metabolites; Gene Clusters; Galaxy; Workflows; Metagenomics.

References:
[1] The Galaxy Community, Nucleic Acids Research, vol. 50, no. W1, pp. W345–W351, Jul. 2022, doi: 10.1093/nar/gkac247.
[2] “Galaxy | Europe.” Accessed: Nov. 22, 2023. [Online]. Available: https://usegalaxy.eu/
[3] K. Blin et al., Nucleic Acids Research, 2023; 51: W46–W50
[4] Q. Gu et al., PLOS Computational Biology 2021;17: e1009014
[5] S. A. Bray, X. Lucas, A. Kumar, and B. A. Grüning, Journal of Cheminformatics 2020;12:40
[6] “Microbial data analysis in Galaxy.” Accessed: Nov. 22, 2023. [Online]. Available: https://galaxyproject.org/projects/microbial/
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[8] J. C. Navarro-Muñoz et al., Nat Chem Biol 2020; doi: 10.1038/s41589-019-0400-9.
[9] V. Pascal Andreu, H. E. Augustijn, K. van den Berg, J. J. J. van der Hooft, M. A. Fischbach, and M. H. Medema, mSystems, vol. 6, no. 5, p. 10.1128/msystems.00937-21, Sep. 2021, doi: 10.1128/msystems.00937-21.

OP05: Molecular docking and simulation studies of hippophaenin-A against penicillin-binding proteins of foodborne pathogenic bacteria

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Background: Bacteria are the leading cause of foodborne diseases. Natural compounds having antimicrobial action can inhibit the growth of harmful bacteria, hence enhancing food safety. Several investigations have also demonstrated that tannin and pure tannin compounds derived from plant extracts have antimicrobial properties. Peptidoglycan is one of the major components of the bacterial cell wall which is essential for bacterial growth. Hence targeting the penicillin binding proteins (PBPs) in the peptidoglycan synthesis pathway is a promising strategy to inhibit the growth of pathogenic bacteria. Hippophaenin-A is one of the less explored tannins found in the *Hippophae rhamnoides* (sea buckthorn) plant. Therefore, hippophaenin-A was subjected to computer simulation to determine the mode of growth inhibition against eight PBPs found in the foodborne pathogenic bacteria.

Methods: MEGA 11.0 software was used to construct the phylogenetic tree of PBPs' sequences utilized in this study. 3D models of PBPs were retrieved from AlphaFold2 Protein Structure Database and analyzed using validation tools. Molecular docking was performed using AutoDock Vina software to determine the binding affinity and molecular interactions of hippophaenin-A and chloramphenicol (reference inhibitor) in the active sites of PBPs. Molecular dynamics simulations (MD) were carried out for 50 ns for each top docking complex and native PBPs of foodborne pathogenic bacteria. The hippophaenin-A was further assessed for physicochemical, pharmacokinetic and toxicity (ADME/T) properties.

Results: The computational investigations of hippophaenin-A demonstrated significant binding affinity and stability with the transpeptidase and transglycosylase catalytic sites of PBPs indicating that the antibacterial activity of hippophaenin-A may be due to PBPs' inhibition. It also displayed favourable physicochemical and ADME properties. Moreover, the toxicity predictions revealed that there was no safety concern to consumers from ingesting hippophaenin-A.

Conclusion: Therefore, further studies on hippophaenin-A will be an insight to develop it as a natural antibacterial agent for food preservation.

Keywords: Foodborne pathogenic bacteria; Hippophaenin-A; Molecular docking; Molecular dynamics; Penicillin binding proteins

OP06: Insight of halimane diterpenoids targeting *Mycobacterium tuberculosis*: virtual screening, DFT, drug-likeness, and molecular dynamics approach

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[2] Department of Chemistry, University of Douala, Douala, Cameroon
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Background: Research on the ethnobiological activity of *Croton sylvaticus* shows that South African traditional healers used this plant to treat Tuberculosis (TB) and mental disorders [1]. These findings are proof of the double competence of these extracts from the stem bark as a tonic and as a therapeutic agent for TB. In addition, the requirements for the incorporation of diastereomers of the same halimane diterpenoids into other halimane diterpenoids in clearly defined ratios block the phagolysosome maturation and macrophage phagocytosis in human cells [6]. For instance, the compound tuberculosinol can be added in the proportion (1:1) to the mixture of the diastereoisomers isotuberculosinol (*R*) and isotuberculosinol (*S*) in turn in the proportion (1:3) [2]. Minor studies on the stereo-clarification of halimane diterpenoids discovered to date have been carried out by Roncero et al [3]

Methods: To design novel antituberculosis (anti-TB) drug agents against *Mycobacterium tuberculosis* (Mtb), we have built a molecular library around 42 Halimane Diterpenoids isolated from natural sources. Two Mtb enzyme drug targets (Mtb Mycothiol S-transferase and Mtb Homoserine transacetylase) have been adopted. The pharmacological potential was investigated through molecular docking, molecular dynamics simulation, density functional theory (gas phase and water), and ADMET analysis.

Results: Our results indicate that (2*R*,5*R*,6*S*)-1,2,3,4,5,6,7,8-octahydro-5-((*E*)-5-hydroxy-3-methylpent-3-enyl)-1,1,5,6-tetramethylnaphtha-lene-2-ol (compound **20**) has displays higher docking score with each of the selected drug targets. In addition, this molecule exhibits satisfactory drug potential activity and good chemical reactivity. Its improved kinetic stability in the Mtb Mycothiol S-transferase enzyme reflects its suitability as a novel inhibitor of Mtb growth.

Conclusion: Further studies can be carried out, such as in vitro and in vivo evaluations are recommended.
Keywords: antituberculosis druglikeness; density functional theory; halimane diterpenoids; molecular docking; molecular dynamics simulation.

References:

[1] A. G. Stafford, P. Pedersen, A. Jäger, J. Van Staden. South African Journal of Botany, **2007**, 73(3), 384-390.
[2] T. Hoshino, C. Nakano, T. Ootsuka, Y. Shinohara, T. Hara. Organic & Biomolecular Chemistry, **2011,** 9(7), 2156–2165.
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YI01: Transcription factor binding site detection for regulatory and functional predictions of biosynthetic gene clusters

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Background: Actinobacteria are known as Nature's medicine makers, to reflect their exceptional ability to produce a wide range of specialized metabolites, including a plethora of antibiotics and anticancer compounds. However, many of these metabolites are not produced under standard laboratory conditions as cognate environmental cues are lacking. The genes that are responsible for the production of these metabolites are often clustered into so-called biosynthetic gene clusters (BGCs). We aim to uncover the triggers that elicit the expression of poorly expressed or silent BGCs. The signals that cause expression of BGCs act through DNA *cis*-regulatory elements where transcription factors (TFs) can bind. Identifying these so-called transcription factor binding sites (TFBSs) is crucial to reconstruct the transcriptional regulatory networks [1].

Methods: In this work, we applied regulation-based genome mining to infer function of BGCs. Specifically, we utilized our recently developed tools MiniMotif (unpublished) and the TFBS Finder module of antiSMASH [2] for TFBS detection. These modules integrate data from the LogoMotif database (unpublished), which contains a comprehensive collection of experimentally validated TFBSs in Actinobacteria.

Results: To illustrate the value of this regulation-based genome mining approach in inferring BGC function, we combined co-expression data and TFBS predictions of the iron-dependent repressor DmdR1, leading to the discovery of a previously undetected siderophore-associated BGC in *Streptomyces coelicolor*. Metabolomic profiling of knockout mutants, wherein the novel siderophore cluster genes were omitted, shows the absence of acyl-capped desferrioxamine variants under low-iron conditions. This finding connects the cluster to iron-acquisition pathways and proves the usability of regulatory information to infer BGC function.

Conclusion: We anticipate that regulation-based genome mining will serve as an starting point for systematically exploring, prioritizing, and inferring the function of unknown biosynthetic gene clusters in strain collections, as exemplified by the discovery of a novel DFO related BGC.

Keywords: regulation-based genome mining; transcription factor binding sites, regulatory networks; gene expression; biosynthetic gene clusters.

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YI02: BitterMasS: predicting bitterness from mass spectra

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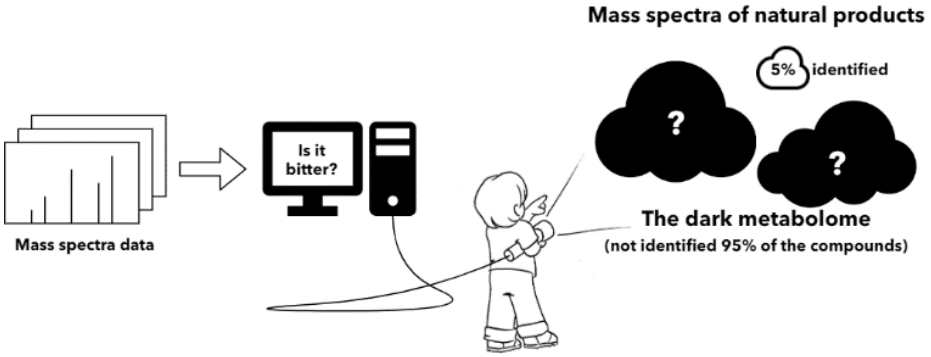
Background: Though bitterness is often assumed to help living organisms avoid toxic compounds in food, studies by the Niv lab [1] have shown that bitterness is not a reliable marker of toxicity. Many natural products taste bitter but have health benefits (e.g., green tea). In addition, perception through the sense of smell is a more reliable marker of toxicity. However, unpleasant odors are still most often associated with bitter taste [2]. Previous work in the Niv lab used chemical structures to predict which molecules may elicit bitter taste in humans, and suggested that above 77% of natural products [3] and 7% of the human metabolome (unpublished) have some bitterness. However, the vast majority (95%!) of the molecules in natural products and in human metabolism have not been identified and have mass spectra that was not assigned to chemical structures (the dark metabolome). It was hypothesized that metabolome can be classified to bitter and non-bitter based on mass spectra, without the need to assign spectra to chemical structures.

Methods: For this reason, it was developed the BitterMasS tool, a machine learning classifier that predicts the probability of a compound having bitterness based on its mass spectrum. The MassBank database was used as a source of experimental mass spectra.

Results: On the test set BitterMasS achieves a balanced accuracy of 0.75 and an F1-score of 0.85. Tests on an external set, which did not participate in model training, showed that the model was effective for a wide range of chemical classes as well as a variety of sources, which were natural products.

Conclusion: BitterMasS will be useful for the food industry to optimize the flavor of natural products. By capturing spectra through a liquid or gas chromatography process paired with a mass spectrometer, BitterMasS will be able to label bitter fractions that require removal or modification to improve the flavor of the source product.

Keywords: Bitterness, Machine learning, Mass spectrometry, Natural products



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YI03: Bio-inspired synthesis, characterization and biomedical applications of optimized silver nanoparticles functionalized with *Ceiba pentandra* (L.) Gaertn. (Kapok tree)

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Background: Malaria control is currently threatened by the emergence of drug-resistant parasites and insecticide-resistant mosquito vectors [1]. Here, silver nanoparticles using *Ceiba pentandra* (CP–AgNPs) were synthesized and their hemocompatibility and lethal activities against *Plasmodium falciparum* (*Pf*) and three mosquito species of medical importance (*Aedes aegypti*, *Culex quinquefasciatus* and *Anopheles stephensi*) were evaluated.

Methods: Crude extract of *C. pentandra* leaves (CP–CE) was prepared, screened for phytochemical composition by gas chromatography coupled with mass spectrometry, and used for CP–AgNPs synthesis and optimization. Standard techniques and protocols were used to characterize the optimized CP–AgNPs and to perform biological assays [2, 3].

Results: UV–Visible spectroscopy revealed a strong surface plasmon resonance at 430 nm. Three main compounds namely 2-Hexadecen-1-ol, 3,7,11,15-tetramethyl-, [R-[R*,R*-(E)]]- (22.3%), Lup-20(29)-en-3-one (11.4%), and 2,3-Dihydro-benzofuran (8.1%) were found in the extract. The optimized CP–AgNPs were predominantly spheroidal, stable, polycrystalline, and coated with several phytochemical compounds (e.g., terpenoids, alkaloids, phenols). The CP–AgNPs were aggregated with mean size of 9.45 nm. CP–AgNPs exhibited good hemocompatibility (250 µg/mL < HC_{50} < 500 µg/mL). CP–AgNPs had high lethal activity on chloroquine-sensitive *Pf* malaria strain (3D7) and chloroquine-resistant *Pf* malaria strain (RKL9) with IC_{50} of 9.71 µg/mL and 15.57 µg/mL, respectively. The CP–AgNPs were most toxic against *An. stephensi* (LC_{50} = 13.48 µg/mL).

Conclusion: Green AgNPs could be an interesting tool for discovery and development of ecofriendly and effective antimalarial drugs and insecticides.

Keywords: biological activities; *Ceiba pentandra*; characterization; green nanoparticles; optimization.

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YI04: *In Silico* search for potential α-amylase inhibitors for management of type 2 diabetes mellitus

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Postprandial hyperglycemia is a metabolic disease characterized by high blood sugar levels in the body. It is currently associated with long-term health burden and significant financial constraints. Globally, over 463 million people had Type 2 Diabetes Mellitus by 2017 and the number is anticipated to double in the next two decades [1]. Addressing this issue by targeting α-amylase enzymatic activity to delay glucose absorption is crucial [2]. However, current antidiabetic drugs often have adverse effects [3]. Computer-aided drug design (CADD) was employed in this study, in finding a potential alternative inhibitor for α-amylase. Two molecules NPC204580 (-14.46 kcal/mol) and NPC137813 (-12.56 kcal/mol) were identified as potential inhibitors for α-amylase by screening the Natural Products Activity and Species database (NPASS). The two molecules displayed strong binding energies and significant interactions with important amino acid residues in the active site of the receptor, as confirmed by molecular docking scores. Stability on active sites and favorable pharmacokinetics/toxicity profiles suggest their potential as T2DM therapeutics. Further investigation such as *in-vivo* and *in-vitro* is warranted to validate their efficacy and safety. These findings underscore the potential of CADD in drug discovery and highlight these compounds as promising candidates for managing postprandial hyperglycemia.

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YI05: Design, synthesis, biological, and computational screening of novel oxindole derivatives as inhibitors of Aurora A kinase and SARS-CoV-2 spike/host ACE2 interaction

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Cancer is a life-threatening disease that kills millions of people each year and in spite of the best efforts, it continues to resist full control and eradication [1]. Interestingly, the overexpression of Aurora kinases and their association with genetic instability and aneuploidy in tumours suggests that a wide range of cancers could respond therapeutically to inhibitors of the Aurora kinases [2]. During the outbreak of COVID-19 in late 2019, there was widespread interest in the repurposing of most anticancer drugs as potential inhibitors of SARS-CoV-2 spike and host ACE2 interactions as a strategy to prevent viral transmission [3]. The isatin-privileged scaffold, found in a broad range of natural and synthetically derived pharmacologically active compounds having antiviral, and anticancer can be modified at the N-1, C-3, C-4, C-5, and C-7 positions with the N-1, C-3, and C-5 positions being the most favorable for activities [4]. This work is meant to affirm the activities of isatin analogues as inhibitors of both Aurora A kinase, and SARS-CoV-2 spike and host ACE2 interactions and to establish their mechanisms of action as well as their structure-activity relations. Several analogs of isatin hybrids have been synthesized and characterized, and their inhibitory activities established as inhibitors of both Aurora A kinase and SARS-CoV-2 spike/host ACE2 interactions. Amongst the synthesized isatin hybrids, compounds **6a, 6f**, **6g,** and **6m** exhibited Aurora A kinase inhibitory activities (with IC50 values <5 μM) while compounds **6g** and **6i** showed activities in blocking SARS-CoV-2 spike with the ACE2 protein (with IC50 values in the range <30 μM). Compounds **6f**, **6g** and **6i** were both capable of inhibiting spike/ACE2 fusion and blocking Aurora A kinase. Pharmacophore profiling indicated that compound **6g**, tightly fits Aurora A kinase and SARS-CoV-2 pharmacophore while **6d** fits SARS-CoV-2 and **6l** Aurora A kinase. This work is a proof of concept that most existing cancer drugs possess antiviral properties. Molecular modelling showed that the active compound for each protein adopted different binding modes, hence interacting with a different set of amino acid residues in the binding site. The weaker activities against spike/ACE2 could be explained by the small sizes of the ligands that fail to address the important interactions for binding to the angiotensin II receptor site.

Keywords: ACE2; Aurora A kinase; SARS-CoV-2; spike/ACE2 interactions.

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YI06: *In silico* anti-Alzheimer potential of bioactive compounds in fungi from the African Natural Products Database

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Research into treatments for Alzheimer's has led to several thousand bioactive compounds being tested in clinical trials, of which over 400 have failed. Given the exponential increase in the number of cases, it makes sense to intensify the search for new anti-Alzheimer's compounds. To this end, bioactive compounds from fungi are candidates for the treatment of Alzheimer's disease (AD). This work presents the anti-Alzheimer's potential *in silico* of fungi compounds contained in the African Natural Products Database (ANPDB) capable of crossing the blood-brain barrier (BBB). A virtual search for compounds of interest in ANPDB was carried out, during which 17 fungal families were identified and 91 bioactive compounds characterized. Among these molecules, those with have a log BB>0.3 in the pkCSM server were selected. Following this, a literature search using references on compelling compounds not studied in Alzheimer's disease was also selected. Conformational site analysis and docking parameters such as binding energy, and interaction profiles with AD target residues were determined. the selected compounds were: (R)-5-(1- hydroxybutyl)-4-methoxy-6-methyl-2H-pyran-2-one, Diorcinol, Elgonene B and H, Ergosta-7-en 3beta-ol and Novae-zelandin. Ergosta-7-en-3beta-ol scored better than donepezil on BuchE. This interacts with His 438 of the catalytic triad, Trp 82 of the anionic site, and Tyr 332 of the peripheral site BuchE. Ergosta-7-en-3beta-ol, Elgonene B and H have higher docking scores on β-secretase. These and diorcinol also showed better score with GSK 3β. This study shows that ergosta-7-en 3beta-ol, Elgonene H and B and diorcinol have multi-targeted therapeutic potential for the treatment of AD.

Keywords: fungi compounds, ANPDB, *in silico*, AD, BBB

YI07: Targeting the intra-erythrocytic life cycle of the malaria parasite to identify starting points for antimalarial drug discovery from *Drymaria cordata and Macaranga monandra*

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Background: The outbreak and spread of parasite strains less sensitive to artemisinin derivatives and the failure of treatment with artemisinin-based combination therapies underline the emergency of searching for new drugs against malaria. However, the intra-erythrocytic life cycle of the parasite is responsible for the clinical manifestations and represents a crucial target for the development of new antimalarial drugs to relieve the symptoms of the disease. Medicinal plants, which have long been used to cure various diseases, were reported to possess several antimalarial bioactive secondary metabolites. Therefore, the general objective of this work was to target the intra-erythrocytic life cycle of the malaria parasite to discover new drugs from *Drymaria cordata* and *Macaranga monandra*, two plants traditionally used in Cameroon for the treatment of malaria.

Methodology: Aqueous, methanolic, ethanolic and hydroethanolic extracts of the whole plant of *D. cordata* and the bark of *M. monandra* were tested *in vitro* against chloroquine-sensitive (Pf3D7) and multi-drug resistant (PfDd2) strains of *Plasmodium falciparum* using the SYBR Green-I test. Subsequently, the effects of active extracts on erythrocyte membrane integrity and on viability of the Vero cell line were evaluated by the spectrophotometric method. The most active and selective extract was selected for bio-guided fractionation. Inhibition kinetics and action specificity of promising fractions on the intra-erythrocytic development cycle of *P. falciparum* were studied.

Results: Only the ethanolic extract of *D. cordata* showed good antiplasmodial activity (IC_{50} PfDd2:18.9 µg/ml; IC_{50} Pf3D7:24.51 µg/ml) while all the extracts of *M. monandra* showed promising antiplasmodial activities (IC_{50} < 8 µg/ml). All active extracts showed no haemolytic or cytotoxic effects. Promising ethyl acetate (IC_{50} PfDd2: 0.60 µg/ml, IC_{50} Pf3D7: 3.42 µg/ml) and n-butanol (IC_{50} PfDd2: 0.92 µg/ml, IC_{50} Pf37D: 2.46 µg/ml) fractions from *M. monandra* bark methanolic extract (IC_{50} PfDd2:2.46 µg/ml; IC_{50} Pf3D7:1.02 µg/ml) have proved to be fast-acting, inhibiting ring development, inducing selective lysis of parasitized red blood cells harboring trophozoites, and blocking the release of new merozoites. Qualitative analysis of this extract revealed the presence of pharmacologically active phytochemicals such as phenols, flavonoids, tannins, anthraquinones, terpenoides and anthocynins.

Conclusions: further investigation of the ethyl acetate and n-butanol fractions from *M. monandra* bark methanolic extract could reveal powerful starting points for antimalarial drug discovery.

Keywords: *Plasmodium falciparum*, *Drymaria cordata*, *Macaranga monandra*, fractionation, mode of action

YI08: Chemical composition of some aromatic plants and insecticidal activities on *Necrobia rufipes*, an insect infesting smoked fish

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Background: Fish is recognized for its nutritional value. However, it is an easily perishable food. To preserve these qualities after capture, smoking is the most used method in Cameroon **(**. However, despite processing, its shelf life remains short, this is mainly due to the proliferation of insects. To control their harmful effects, synthetic insecticides are used. These, although effective, have drawbacks. To overcome these limitations, researchers are moving towards alternatives that respect the environment and human health, such as essential oils.

Methods:The leaves of *Lippia multiflora, Lantana camara, Eucalyptus citriodora, Eucalyptus saligna* were collected in the city of Douala. The essential oils were extracted by hydrodistillation and analyzed for chemical composition using gas chromatography coupled with mass spectrometry (GC-MS). The insecticide tests were carried out by the contact-inhalation method on the insect *Necrobia rufipes*.

Results: The GC–MS analysis allowed the identification of volatile components, the majority of which are essential oils*: L.multiflora*: Citral (26.25%), Geraniol (25.60%), *L.camara*: Caryophllene (28.95%), Eucalyptol (18.25%), *E.citriodora:* Eucalyptol (17.25%),Limonene (14.74%), *E.saligna* : αTerpineol (24.13%), Eucalyptol (17.49%). The insecticidal activities of essential oils were obtained according to the lethal dose 50 or 4.5ul; 12ul;12ul; 14ul respectively for *L. multiflora, L. camara, E. citriodora, E. saligna.*

Conclusions: The results obtained from this study revealed the insecticidal bioeffectiveness of essential oils, the most effective of which is *L.multiflora*. These insecticidal properties are due to its richness in chemical constituents with strong insecticidal potential. *L. multiflora* could therefore be a suitable topical agent to control *Necrobia rufipes* infestations and could be useful for commercial formulations.

Keywords: insecticidal, *Lippia multiflora, Lantana camara, Eucalyptus citriodora, Eucalyptus saligna*

YI09: Design and implementation of a unified version of the African Natural Products Database (ANPDB)

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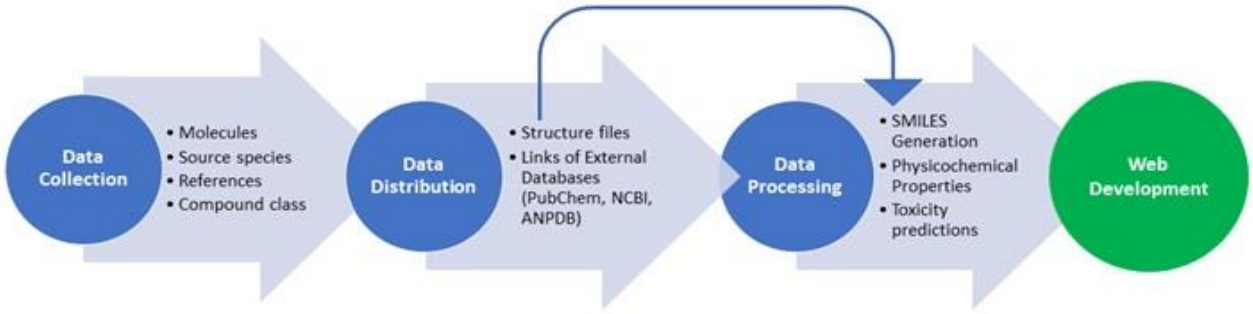
As an ongoing project, we are developing a database of natural products derived from African natural sources. After careful data search, collection, and curations, SMILES strings of compounds were obtained directly from PubChem and from mol structures generated using in-house Python scripts. The pharmacokinetic profile of compounds such as Lipinski's Rule of Five, and toxicity predictions will be computed using Computed Aided drug design tools like QikProp and SWISSADME to assess their drug-likeness [3]. The dataset (ANPDB) generated would be useful to generate new scaffolds which would lead to new compounds and their biological activities would be evaluated against different targets of SARS-CoV-2 and HIV) or the discovery of synthetic routes toward secondary metabolites.

Keywords: ANDPB; antiviral compounds, virtual screening,



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YI10: Can AI revolutionize natural products research? the genus *Vernonia* compounds as a case study

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Secondary metabolites are crucial for treating infections; however, many are underexplored due to the expansion of natural product databases [1]. Similarly, interest in natural products for drug discovery has declined, primarily due to challenges associated with their isolation, characterization, and synthesis [2]. In response to these challenges, there has been a recent surge in the application of computational approaches to drug discovery. However, these compounds systematized pharmacokinetic and ADMET profiles have been briefly investigated. Therefore, this study evaluated the chemistry and pharmacoinformatics of compounds derived from *Vernonia* species. To achieve this, we complied identified compounds from the literature, and ADMET properties were procedurally determined as described by [3,4]. The data was then retrieved into an Excel spreadsheet and statistically analyzed. The finding revealed that 72.2% of the compounds obey Lipinski's rule of five, 67.4% are within Veber's rule, and 58.8% meet Egan's rule. Notably, no compounds showed inhibition of hERG I, but 31.5% were anticipated to inhibit hERG II. Moreover, 87.3% of the molecules showed no potential for skin sensitivity while 64.3% inhibited high intestinal absorption. In conclusion, phytochemicals of the genus *Vernonia* exhibited physiochemical profiles comparable to those of FDA-approved drugs. This provides a special chance to restore natural products as a significant source of drug discovery while offsetting the inherent limits of natural products.

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YI11: *In silico* analysis of ADME/Tox profile of compounds from *Croton* species

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Croton comprises over 1300 species with >900 phytochemicals and diverse biological activities. In this study, we conducted a comprehensive *in silico* analysis of previously reported *Croton* spp. compounds to identify potential drug candidates based on their physicochemical and pharmacokinetic properties as described by [1]. This analysis aimed to provide a virtual ADMET profile of these compounds, facilitating the selection of promising leads for further development. Data collection involved a literature survey of the *Crotons* compounds, followed by obtaining their ADMET properties from SwissADME and pkCSM which were then analyzed on the Origin Pro 2023 platform [2]. It was noted that diterpenoids (67.2%), alkaloids (11.1%), sesquiterpenes (4.7%), flavonoids (3.2%), other terpenoids (Sesterterpenoid and triterpenoids; 2.7%), monoterpenoids (1.7%), megastigmane glycosides (2.2%), proanthocyanidins (0.8%), and other assorted compounds (6.4%) make up the total of 900 compounds. The biological activity that was most frequently reported was cytotoxicity (52%) followed by anti-inflammatory actions (13%). Most of these compounds share the same common chemical space with FDA-approved drugs based on principal component analysis. ADME screening indicated that 38% of the *Croton* compounds met the criteria for drug-likeness while toxicity prediction analysis cleared 35.487% as nontoxic. The primary compounds identified as appropriate drug likes included Clerodanes, Abietanes, Kauranes, and Labdanes, with respective ratios of 23.5%, 17.6%, 17.6%, and 11.8%, respectively. The study indicated these as potential druglike compounds from the *Croton* worth further therapeutic screening.

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YI12: Identification of novel Atg3-Atg8 inhibitors using virtual screening for autophagy modulation

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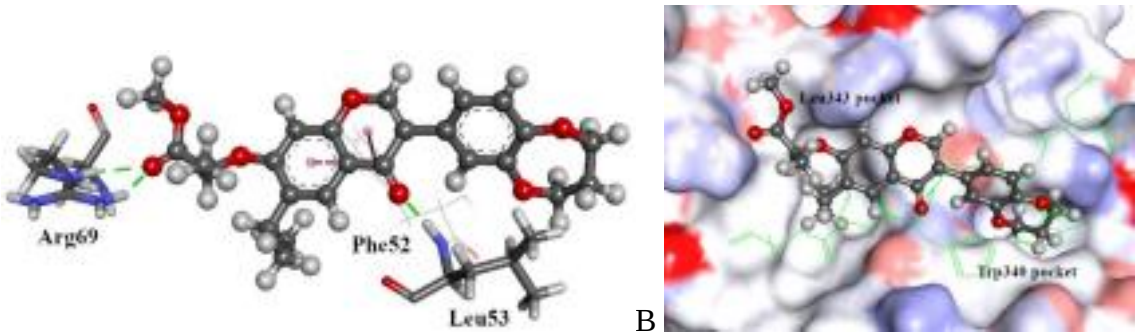
Autophagy (self-eating) is a metabolic process for recycling damaged cellular material, which is captured by autophagosomes and directed to lysosomes for bulk degradation.[1] Autophagy dysfunction is associated with many diseases, such as cancer and neurodegeneration, making the autophagy machinery a potential therapeutic target.[2, 3] A key step in this pathway is the complexation of the ubiquitin-related Atg8 protein family to the Atg3 polypeptide.[4] Virtual high throughput screening in conjunction with MCF7 breast cancer cell line and zebrafish model test has been used to identify Atg3-Atg8 inhibitors consisting of chromones, coumarins and phenyl ketones. Molecular modelling shows that the active ligands form hydrogen bonds with Arg69, Leu53, Phe52. Three hits showed single digit µM IC50 values with AT110, an isoflavone derivative, being the most active at 1.2 ± 0.6 µM. A small molecule non-cytotoxic autophagy inhibitor such as AT110 would open the door for adjunct therapies to bolster many established anticancer drugs, reducing their efficacious concentration and thus limiting undesirable side effects. In addition, since many cancer types rely on the autophagy mechanism to survive a therapeutic regime, recurrence can potentially be reduced. Hence, the discovery of AT110 is an important step in establishing such an adjunct therapy.



A B

Fig 1. The docked pose of AT110 in the complexation site of Atg3-Atg8, as predicted by the ChemScore function. (A) The predicted configuration is shown in the ball-and-stick format and the adjacent amino acid residues are depicted in the stick format except the Phe52 amino acid residue is shown in the line format for clarity. Hydrogen bonds are shown as green lines while π-π stacking is shown in pink (B) The Atg8 protein surface is rendered; blue depicts regions with a partial positive charge on the surface; red depicts regions with a partial negative charge and grey shows neutral areas. The co-crystalized Atg3 is depicted in green inline format.

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HS01: Exploring antimalarial drug discovery through cheminformatics and QSAR modeling

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Quantitative Structure-Activity (or -Property) Relationship (QSAR/QSPR) models have matured into indispensable tools in drug discovery, enabling scientists to predict biological activities and physicochemical properties of compounds based on their molecular structures. By bridging the gap between chemistry and pharmacology, these computational models accelerate the identification and optimization of potential drug candidates. In Africa, where neglected tropical diseases affect more than one billion people, efficiently leveraging such resources would provide cost-efficient solutions to speed up the discovery and development of urgently needed cures. Upon providing a brief overview of the applications of cheminformatics and machine learning in drug discovery, this hands-on workshop will guide participants through various steps towards the development of high-quality QSAR models to predict the antimalarial activity of small molecules. These will cover, among others:

1) the exploration of data acquisition and curation strategies, unraveling the complexities of chemical information and molecular structures;

2) data featurization techniques; and

3) the iterative process of model building, validation, and interpretation. The session will culminate in a comprehensive discussion on model design and best practices, empowering attendees to assess the reliability and applicability of their QSAR models. Participants will gain practical skills that can be directly applied to their research, addressing specific challenges of drug discovery.

Target audience
Beginners or professionals in the field of (bio-)chemistry, biology, data science, or any related field, with interest in cheminformatics and predictive modeling for drug discovery.

Prerequisites
[1] Basic understanding of chemistry concepts.
[2] Basic understanding of statistical analysis or machine learning concepts.
[3] Familiarity with molecular structures and chemical descriptors.
[4] Comfortable working with data.
[5] Some experience with (Python) programming or a willingness to learn basic programming concepts

HS02: ProBiS for drug development

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In this lecture, you will gain experience with ProBiS algorithms, databases, and web servers, equipping you with the skills needed to explore, analyze, and interpret protein structures. By converting protein structures into mathematical graphs, ProBiS enables you to apply graph-based algorithms and techniques for in-depth exploration. You will discover how the ProBiS tools facilitate the comparison and analysis of protein structures. By aligning and comparing the graph representations of different proteins, you will uncover invaluable insights into their overall architectures, identifying both similarities and differences. Additionally, you will learn to pinpoint specific regions that exhibit structural variations, enabling you to identify conserved motifs, evolutionary relationships, and crucial structural elements that contribute to the protein's function and dynamics, including drug binding. The insights gained from this approach have far-reaching implications, impacting various fields including drug discovery, bioengineering, and molecular biology.

Figure 1: INSILAB - In silico laboratory for innovation in drug discovery develops ProBiS (protein binding sites) tools.

Keywords: algorithms; binding sites; ligands; prediction; proteins; web servers.

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HS03: Galaxy for Secondary Metabolite Discovery - from isolates to metagenomes - hands-on workshop

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Galaxy [1], is a comprehensive data science and workflow management platform that offers a web-based, intuitive, and user-friendly interface to command-line tools. It automates computation and data provenance management while transparently scheduling workflows, making it easier for scientists to perform complex bioinformatic tasks. Users without access to computing facilities can perform their analysis on public Galaxy instances, such as Galaxy Europe [2], that allow running tools that require large computational resources for everyone. Various tools exist for common tasks in metabolite discovery, such as antiSMASH [3] as well as complete tool libraries for statistics, machine learning [4] and cheminformatics [5]. In recent years, the metagenome tool stack of Galaxy has grown to more than 200 tools [6], providing the possibility to combine metabolite discovery and metagenome analysis workflows, to gain an improved understanding of community dynamics. Galaxy is also connected to large data sources, such as the MGnify database [7], that provides access to metagenome data that was analyzed by standardized workflows and includes taxonomic classification as well as gene cluster predictions. To further extend these analysis capabilities, the Freiburg Galaxy Team is currently working on the integration of dedicated tools, such as BIG-SCAPE [8] and BIG-MAP [9], that allow for gene clusters analysis on metagenomic scale. Here, we would like to present the current capability of Galaxy for secondary metabolite discovery; introduce the microbial community; explain how researchers can get involved; and the envisioned developments. The hands-on session guides users through the basics of Galaxy and introduces some examples, that can be used as a starting point to develop complex secondary metabolite discovery and joint metagenome analysis workflows. The participants can follow the hands-on session on the public Galaxy Europe instance.

Keywords: Secondary Metabolites; Gene Clusters; Galaxy; Workflows; Metagenomics.

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HS04: Identification of bioactive natural products by virtual screening

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In this hands-on session, participants will explore the web tools that permit the search of databases, including similarity and sub-structure searching for privileged scaffolds. After you have been introduced to the natural product databases from African sources, their contents, compound classes and potential for lead compound discovery, the last session (about 50 minutes) will introduce state-of-the-art computational techniques used in lead compound identification from electronic databases, e.g. molecular docking and pharmacophore-based searching. In this section you will be introduced to the approaches used to perform *in silico* screening of libraries containing natural products against a main protease for the COVID-19. You will also be briefly introduced to other sophisticated tools like molecular dynamics and metadynamics, just on the fly. Participants will learn how to perform virtual screening from large libraries (focusing on natural products libraries from African sources), e.g. the South African Natural Compounds Database (SANCDB - https://sancdb.rubi.ru.ac.za/) [1], which is is a collection of 1,012 compounds derived from South African natural sources. Since its inception in 2015, the database has been used for various machine learning and *in silico* virtual drug screening studies with a recent study identifying several potential hits against severe acute respiratory syndrome coronavirus 2 (SARS-COV-2). As part of a recent update, a unique feature incorporating the compound dataset analogs from two leading commercial databases (Molport and Mcule) was included. The feature will not only allow users to explore a larger chemical space during screening but also allow them to seamlessly purchase compounds for their biological studies. Participants will be introduced to the database with emphasis on how they can obtain compounds for both their virtual screening and biological studies. The second part of the session (approximately 20 minutes) will focus on natural products databases originating from the regions of Northern [2] and East Africa [3] (http://africancompounds.org/anpdb/).

Keywords: lead identification; natural products; molecular docking; virtual screening; drug discovery.

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Part V: Downloads and Supplementary Materials

antiSMASH:

https://antismash.secondarymetabolites.org

antiSMASH DB:

https://antismash-db.secondarymetabolites.org

MIBiG repository:

https://mibig.secondarymetabolites.org

Secondary Metabolite Bioinformatics Portal:

https://www.secondarymetabolites.org

CRISpy-web:

https://crispy.secondarymetabolites.org

PatScanUI:

https://patscan.secondarymetabolites.org

Uresearcher.com Project:

https://uresearcher.com/project/build-machine-learning-bioactivity-predictor-python

https://drive.google.com/drive/folders/1kKGBT3P1yQ0BaN4o_FbzoA9-rvj1aIBO?usp=sharing

ChemBL Database:

https://uresearcher.com/article/how-to-get-started-chembl-database

ANPDB Database:

http://african-compounds.org/anpdb/

SANCDB Database:

https://sancdb.rubi.ru.ac.za/

ProBiS Tools:

http://probis.cmm.ki.si/

BitterDB:

https://bitterdb.agri.huji.ac.il/dbbitter.php