Book of Abstracts

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Contents

COVER PAGE **1**

Part I: About the Workshop **5**

I.1. What to expect 7

I.2. Audience 7

I.3. Registration 7

I.4. Abstract submission 7

I.5. Keynote presentations/Round table discussions 7

I.6. Hands-on session 8

I.7. Oral presentations 8

I.8. Poster/flash presentations 8

I.9. Time zone 8

I.10. Lecture option and web platform 8

I.11. Certificate of participation 8

I.12. Cost of participation 9

I.13. Language of workshop 9

I.14. Workshop materials 9

I.15. Zoom link 9

Part Part II: Workshop Programme **9**

II.1. Day 1 11

II.2. Day 2 11

II.3. Day 3 11

Part III: Abstracts **12**

KL01: Allosteric Modulator Identification from South African Natural Compounds Database (SANCDB) against SARS-CoV-2 Mpro Protein in the Presence of its Evolutionary Mutations 14

KL02: Tools for Innovative Drug Design 15

KL03: Developing the Tools to Digitize the Chemistry of Microbes 16

OP01: Galaxy Framework Exordium 17

OP02: Computational Investigation of Natural Products as Lead Compounds: Drug Repurposing using Clustering and Fingerprinting Algorithms 18

OP03: In Silico and in Vitro Studies of Cytotoxicity and the Mode of Action of Dichapetalins A and M 19

OP04: Molecular Insight into the Interaction between the Spike Protein of the Wildtype, Delta and Omicron SARS-CoV-2 and the Human Angiotensin Converting Enzyme 2 (hACE2): Potential for the Design of Fusion Inhibitors 20

OP05: Cheminformatics Analysis of Ring Systems in Natural Products 21

OP06: Ersilia, a Hub of Open-Source AI/ML Models for Drug Discovery and Global Health 22

OP07: A Taste of Nature - Predicting and Modulating Bitterness 23

OP07-2: Evaluation of Trypanocidal Activity and Mode of Action of a Steriod from Vitex simplicifolia Leaves 24

OP08: In Silico Polypharmacology and Efficacy of Natural Products 25

OP09: Insights into Intramolecular Interactions of Transition Metal-Bis-(N-Heterocyclic Carbene) Complexes and Topological Unraveling the C-H Bond Activation from QTAIM/ELF/EDA/NBO and BET Theory 26

OP10: Trigonelline: A Promising Compound for The Treatment of Alzheimer's Disease . 27

OP11: Search for Schweinfurthins and other Secondary Metabolites from Macaranga Occidentalis (Euphorbiaceae) and Evaluation of Possible Anticancer Activity 28

OP12: Molecular Docking and In Silico ADMET Predictions of Amodiaquine Derivatives as Antimalarial Agents 29

OP13: A Molecular Investigation of the Solvent Influence On Inter- and Intra-Molecular Hydrogen Bond Interaction of Linamarin 30

OP14: Hepatoprotective Effects of Extracts, Fractions and Compounds from Pentaclethra macrophylla Benth against Experimental Hepatotoxic Models 31

HS01: Genome Mining using antiSMASH, and the antiSMASH and MIBiG databases . . 32

HS02: Building a Machine Learning-Based Bioactivity Predictor 33

HS03: Visualization of RNA-Seq with Galaxy Framework 34

HS04: Virtual Screening for the Fast and Cheap Identification of Bioactive Natural Products 35

Part IV: Speakers 36

IV.1. Jude Betow 37

IV.2. Ozlem Tastan Bishop 37

IV.3. Kai Blin 38

IV.4. Mary Anti Chama 39

IV.5. Ya Chen 40

IV.6. Lucie Karelle Djogang 41

IV.7. Pieter Dorrestein 42

IV.8. Miquel Duran-Frigola 43

IV.9. Samuel Ayodele Egieyeh 44

IV.10. Mai M. Farid 45

IV.11. Akachukwu Ibezim 46

IV.11. Dusanka Janezic 47

IV.12. Darshana Joshi 48

IV.12. Jutta Ludwig-Müller 49
IV.13. José L. Medina-Franco 50
IV.14. Pankaj Mishra 51
IV.15. Thommas Mutemi Musyoka 52
IV.16. Masha Niv 53
IV.17. Fidele Ntie-Kang 54
IV.18. Jean Moto Ongagna 55
IV.18. Victor Chukwudi Osamor 56
IV.19. Lucas Paul 57
IV.20. Daniel Madulu Shadrack 58
IV.21. Pierre Valery Kemdoum Sinda 59
IV.22. Kiran Kumar Telukunta 60
IV.23. Tilmann Weber 61

Part V: Downloads and Supplementary Materials 62

V.1. antiSMASH 64
V.2. antiSMASH DB 64
V.3. MIBiG repository 64
V.4. Secondary Metabolite Bioinformatics Portal 64
V.5. CRISpy-web 64
V.6. PatScanUI 64
V.7. Uresearcher.com Project 64
V.8. ChemBL Database 64
V.9. ANPDB Database 64
V.10. SANCDB Database 64
V.11. ProBiS Tools 64
V.12. BitterDB 64

Part 1: About the Workshop

FREE ONLINE WORKSHOP ON SECONDARY METABOLITE DISCOVERY (9th-11th MARCH 2022)

CAiSMD 2022: Computational Applications in Secondary Metabolite Discovery

All the workshop related links you will find under the link
https://indiayouth.info/index.php/caismd/workshop

What to expect

In 3 days, the participants of this online workshop will take a survey of modern computer-based approaches for exploring natural products (or secondary metabolites) discovery in the omic age. Selected experts will give keynote lectures, hands-on sessions, round table discussions, and oral presentations. Selected applicants (mostly early-career scientists and students) will be invited to give oral presentations (15 minutes) and present posters in the form of (5 minutes) flash presentations.

Audience

M.Sc. and Ph.D. students, postdocs, and early-career researchers interested in bioinformatics, chemoinformatics, natural products chemistry, computational drug design, genomic analysis, with applications in drug discovery.

Registration

Participants should fill out the Registration Form available at the weblink
https://indiayouth.info/index.php/caismd/registration.
Those who plan to do a presentation during the workshop should upload an abstract using the prescribed abstract template. All applications for participation must be received by the deadline on 6th March 2022 by midnight CET.

Abstract submission

Abstract for oral presentations (keynotes, standard oral presentations, and flash presentations) must be received by midnight on 4th March 2022 CET. The final program of the workshop will be published by 6th March 2022.

Keynote presentations/Round table discussions

Selected experts will be directly invited by the organizers. Keynote lectures and round table discussions will last from 30 to 60 minutes.

Hands-on session

Selected experts will be directly invited by the organizers to give lectures and practical sessions on specific software tools for web servers. Each session will last for 90 minutes.

Oral presentations

This will last up to 15 minutes each and will be selected among applicants who submit an abstract using the provided template by the deadline of 4th March 2022 by midnight (CET).

Poster/flash presentations

Selected posters from M.Sc. and Ph.D. students will be presented in 5 min flash presentations. All submissions will be received by the expected deadline (4th March 2022 CET by midnight). Keynote presentations, round table discussions, and hands-on sessions are upon invitation by the workshop organizers. Presentations not accepted as standard (15 minutes) oral presentations will automatically be assigned as flash presentations or rejected.

Time zone

All workshop events follow Central European/West African Time.

Lecture option and web platform

All lecture slides will be uploaded by presenters 24 hours before the workshop and will be available for download by the workshop participants.

Certificate of participation

Participants who attend at least 60% of all lectures and take part in an online post-workshop survey will receive a signed certificate of participation.

Cost of participation

Free of charge

Language of workshop

English

Workshop materials

Book of abstracts, lecture slides, hands-on tutorials, YouTube channel containing videos of lectures.

Zoom link

URL:

https://tu-dresden.zoom.us/j/87496530101?pwd=Zk8veFJITnpienRhS3RlU0pwWXlWZz09

Meeting-ID: 874 9653 0101

Password: !L@#4Q^6

Part II: Workshop Programme

Day 1: 09 March 2022

Time	**Event (Chair: J. Ludwig-Müller)**
01:45 pm	Opening of the Workshop
01:50 pm	KL01 (Ö. Taştan Bishop, 45 min)
02:35 pm	Break
02:45 pm	Parallel Hands-on Sessions (HS01 and HS02, 90 min)
04:15 pm	End of HS01 and HS02
04:25 pm	Announcements and End of Day 1

Day 2: 10 March 2022

Time	**Event (Chair: Ö. Taştan Bishop)**
08:00 am	KL02 (D. Janežič, 45 min)
08:45 am	OP01 (K. K. Telukunta, 30 min)
09:15 am	OP02 (V. C. Osamor, 15 min)

09:30 am: Coffee break (15 min)

Time	**Event (Chair: F. Ntie-Kang / T. M. Musyoka)**
09:45 am	OP03 (M. A. Chama, 15 min)
10:00 am	OP04 (S. A. Egieyeh, 30 min)
10:30 am	RTD01 (All lecturers of day 1 and first part of day 2, 90 min)

12:00 pm: Lunch break (90 min)

Time	**Event (Chair: D. Janežič)**
01:30 pm	OP05 (Y. Chen, 30 min)
02:00 pm	OP06 (M. Duran-Frigola, 30 min)
02:30 pm	OP07 (M. Niv, *replaced* by A. Ibezim, 30 min)

3:00 pm: Coffee break (30 min)

Time	**Event (Chair: J. Ludwig-Müller)**
03:30 pm	Parallel Hands-on Sessions (HS03 and HS04, 90 min)
05:00 pm	End of HS03 and HS04
05:05 pm	Closing remarks of Day 2

Day 3: 11 March 2022

Time	Event (Chair: F. Ntie-Kang)
08:00 am	KL03 (P. Dorrestein, 45 min)
08:45 am	TY (Test yourself exercises from the parallel HS, 45 min)

09:30 am: Coffee break (15 min)

Young Investigators Session (from selected submitted abstracts)

Time	Event (Chair: F. Ntie-Kang / S. A. Egieyeh / T. Weber)
09:45 am	OP08 (D. M. Shadrack, 15 min)
10:00 am	OP09 (J. M. Ongagna, 15 min)
10:15 am	OP10 (M. M. Farid, 15 min)
10:30 am	OP11 (J. Betow, 15 min)
10:45 am	OP12 (L. K. Djogang, 15 min)
11:00 am	OP13 (L. Paul, 15 min)
11:15 am	OP14 (P. V. K. Sinda, 15 min)
11:30 am	RTD02 (J. L. Medina-Franco, 90 min)
1:00 pm	Closing remarks

Hands-on Sessions

Day 1: HS01 K. Blin/T. Weber (Bioinformatics)

Day 1: HS02 P. Mishra (Chemoinformatics)

Day 2: HS03 K. K. Telukunta (Bioinformatics)

Day 2: HS04 D. M. Shadrack/ T. M. Musyoka/ F. Ntie-Kang (Chemoinformatics)

Part III: Abstracts

KL01: Allosteric Modulator Identification from South African Natural Compounds Database (SANCDB) against SARS-CoV-2 M^{pro} Protein in the Presence of its Evolutionary Mutations

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The South African Natural Compounds Database (SANCDB; https://sancdb.rubi.ru.ac.za/) is a referenced database of NPs derived from sources within South Africa [1,2]. Since its establishment, the database has attracted significant interest in diverse domains including natural product research, drug discovery, cheminformatics and machine learning. In the last two years, SANCDB has also been screened by us and others against SARS-CoV-2 drug targets.

This talk introduces some of our novel approaches to computational drug discovery using natural compounds: Identification of allosteric drug targeting sites; searching allosteric modulators via natural compounds, i.e. SANCDB; and understanding the allosteric mechanisms of these modulators in the presence of evolutionary mutations. Our case study, here, is SARS-CoV-2 main protease (M^{pro}).

In this study [3,4], we identified six potential allosteric modulators from SANCDB against M^{pro}. We observed that the stability of the potential hit compounds drastically changed in the presence of some of the mutations. Further, in the presence of some of the mutations, the allosteric communication path between the allosteric ligand binding site and the active site was lost. Collectively, the computational approaches that we established in this study offer routes for novel rational drug discovery methods and provide computationally feasible platforms to identify key functional residues implicated in allosteric signaling in the presence of allosteric modulators.

Keywords: allostery; communication paths; drug discovery; natural products

References:

[1] B. N. Diallo, M. Glenister, T. M. Musyoka *et al*. SANCDB: an update on South African natural compounds and their readily available analogs. *J Cheminform*, **2021**,*13*, 37.
[2] R. Hatherley, D. K. Brown, T. M. Musyoka *et al*. SANCDB: a South African natural compound database. *J Cheminform*, **2015**, *7*, 29.
[3] O. Sheik Amamuddy, R. Afriyie Boateng, V. Barozi V, *et al*. Novel dynamic residue network analysis approaches to study allosteric modulation: SARS-CoV-2 M^{pro} and its evolutionary mutations as a case study. *Comput Struct Biotechnol J*, **2021**, *19*, 6431-6455.
[4] O. Sheik Amamuddy, G. M. Verkhivker, Ö. Tastan Bishop. Impact of Early Pandemic Stage Mutations on Molecular Dynamics of SARS-CoV-2 M^{pro}. *J Chem Inf Model*, **2020**, *60*, 5080-5102.

KL02: Tools for Innovative Drug Design

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We develop new methodological solutions for prediction and study of protein binding sites on the PDB scale, based on graph theoretical approaches, combined with molecular dynamics simulations. A special focus is on the development of new algorithms for the prediction of protein binding sites (ProBiS) and new web tools for modeling of pharmaceutically interesting molecules - ProBiS Tools (algorithm, database, web server). The ProBiS Tools are the first to allow the identification of interactions between protein structures, the prediction of ligand selectivity and binding, and the monitoring of the effects of conserved waters and sequence variants on ligand binding, to surpass human involvement in drug design.

Keywords: algorithms, computer simulations, graph theory, drug development, ProBiS

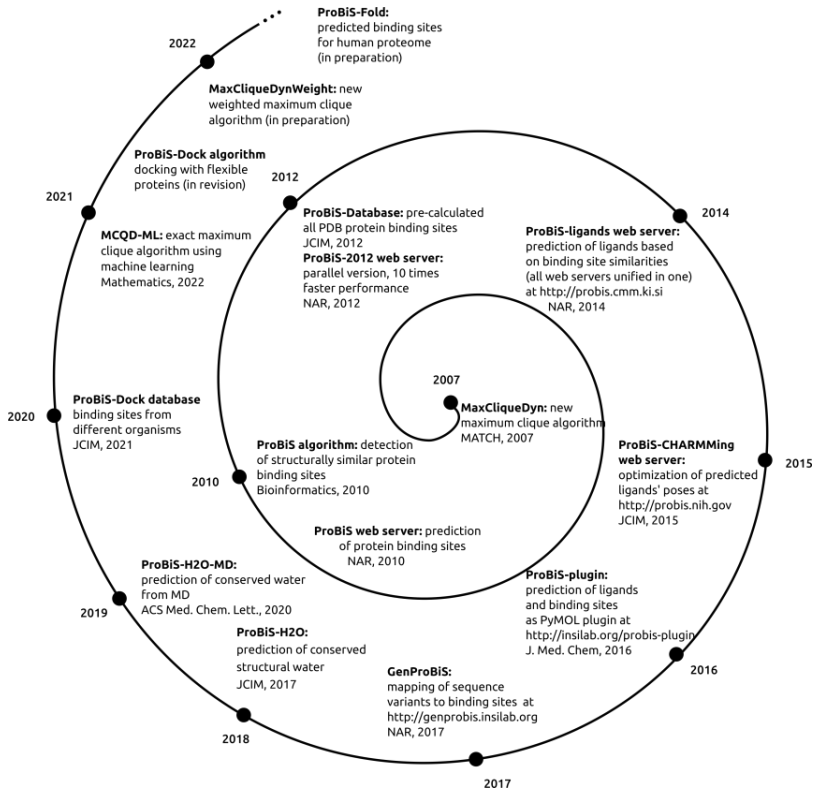

Figure 1: Evolution of the ProBiS Tools

References:
[1] J. Konc, D. Janežič, *Bioinformatics*, **2010**, *26*, 1160–1168.
[2] J. Konc, S. Lešnik, B. Škrlj, D. Janežič, *J Chem Inf Model*, **2021**, *61*, 4097–4107.

KL03: Developing the Tools to Digitize the Chemistry of Microbes

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It is becoming clear that the microbiome plays critical roles in human health but to understand the roles microbes play and their relationship to the chemistries in our bodies is still poorly understood. The University of California - San Diego (UCSD) has recently launched the microbiome center. The Collaborative Mass Spectrometry Innovation Center plays a key and integrated role in this center to begin unraveling the chemistry of the microbiome. In this presentation we will highlight the latest mass spectrometry-based tools, including our crowd source molecular annotation platform and repository scale analysis, to study the chemistry of the diet and microbiome associated with the host (plants, animals, humans) in relationship to ecosystem health information as well as understanding the chemistry of human, environmental or ecological habitats.

Keywords: mass spectrometry; metabolomics: microbiome; molecular annotation.

OP01: Galaxy Framework Exordium

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The Galaxy [1] framework since its start in 2006 has been able to contribute to more than 11,500 publications. The Galaxy ecosystem is instituting the platform for data intensive science research. It also mainly focuses on workflows which bolster drug discovery. Apart from drug discovery supplementing several areas of bioinformatics such as Assembly of genome sequences, Climate data, Computational chemistry, Ecology, Epigenetics, Genome Annotation, Imaging, Metabolomics, Metagenomics, Proteomics, Sequence analysis, Statistics and machine learning, Transcriptomics, Variant Analysis, and Visualization [2]. It also particularly allows the community to develop and contribute to the project under academic Free License 3.0. The oral presentation introduces the Galaxy framework and gives an exordium to your open-source research and opens the door for accelerated research. Subsequently, there will be a hands-on session in the workshop which will guide how to use the Galaxy framework for visualization analysis.

Keywords: framework; galaxy; open-source.

References:
[1] E. Afgan, D. Baker, B. Batut, *et al*., The Galaxy platform for accessible, reproducible and collaborative biomedical analyses: 2018 update, *Nucleic Acids Res*, **2018**, *46*, W537–W544.
[2] A. Syme, N. Soranzo, 2021 A short introduction to Galaxy (Galaxy Training Materials). https://training.galaxyproject.org/training-material/topics/introduction/tutorials/galaxy-intro-short/tutorial.html Online; accessed Wed Mar 07 2022

OP02: Computational Investigation of Natural Products as Lead Compounds: Drug Repurposing using Clustering and Fingerprinting Algorithms

Victor Chukwudi Osamor,[1,*] and Theresa Okediya[1]

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Background: Natural products (NPs) play a significant role in drug discovery and development. Given the remarkable chemical diversity in nature, natural products are considered as a rich reservoir of bioactive compounds with therapeutic potentials. Natural products, with remarkable chemical diversity, have been extensively investigated for their anticancer potential for more than a half-century. Regardless of these achievements, developing bioactive natural products into drugs has remained challenging, in part because of the difficulty in large-scale isolation, mechanistic understanding, and pharmaceutical development. There is a need for a means to pre-sort candidates using computational chemistry and cheminformatics methods. This research work aims to investigate if some set of studied natural compounds can be considered as lead molecules.

Methods: The studied natural molecules were gotten from the African natural compounds database while the traditional drugs were gotten from the PubChem database. A total of 4936 small molecules were used in the experiment, containing 12 existing drugs for cancer and 4924 natural compounds. The ChemmineR cheminformatics package in R was used to generate the fingerprints for each molecule and perform other preprocessing tasks, the molecular similarity between molecules was then calculated using the Tanimoto coefficient with a cutoff of 0.5. For the clustering, the agglomerative hierarchical and K-means clustering techniques were adopted, and the result was visualized using dendrograms.

Result: The dataset was reduced to 482 molecules after conducting the structural molecular similarity measurement. Based on the molecular distances and ward's method, the remaining molecules were grouped into clusters. The result shows that some of the natural molecules are clustered with some existing drugs. The results were consistent with the two clustering techniques used.

Conclusion: Based on the similarity property principle, drugs with similar molecular structures are likely to have the same properties. This may indicate that they have similar properties and can be further tested as potential drug candidates.

Keywords: cheminformatics; clustering; drug discovery; lead molecule; natural products.

OP03: *In silico* and *In vitro* Studies of the Cytotoxicity and the Mode of Action of Dichapetalins A and M

Mary A. Chama,[1] Daniel Ayine-Tora,[1] Lily Paemka,[1] George Yankson,[1] and Andreas Bender[2]

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[2]Department of Chemistry, University of Cambridge, Cambridge, UK
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Background: Dichapetalins A and M are among a class of known triterpenoids isolated from the plant *Dichapetalum madagascariense* Poir (Dichapetalaceae) [1]. The dichapetalins have shown a broad spectrum of biological activities including cytotoxicity to different cancer cell cells [2,3]. The cytotoxicity of of dichapetalins A and M against MCF-7 cells was evaluated to determined possible mode of mechanisms.

Methods: Both dichapetalins were isolated by column chromatography and identified using NMR and Mass spectrometry. The PIDGINv2 [4] was used for target prediction whiles molecular docking was carried out using the GOLD v5.4 software suite. Cytotoxicity measurements were done against the MCF-7 cells via the MTT assay and target validation carried out with expression studies with qPCR.

Results: The IC_{50} of dichapetalin M was higher (4.71 µM and 3.95 µM) for 48 and 72 hrs of treatment, respectively compared to Curcumin with an IC_{50} of 17.49 µM and 12.53 µM for 48hrs and 72hrs of treatment, respectively. *In vitro* expression studies with qPCR confirmed an antagonistic effect of dichapetalin M on PXR (NR112) signaling; supporting the PXR signaling pathway as a possible mode of action of dichapetalin M.

Conclusion: The findings suggest that dichapetalin M could be a lead compound for potential anticancer drug.

Keywords: cytotoxicity; dichapetalin A; dichapetalin M; MCF-7 cells.

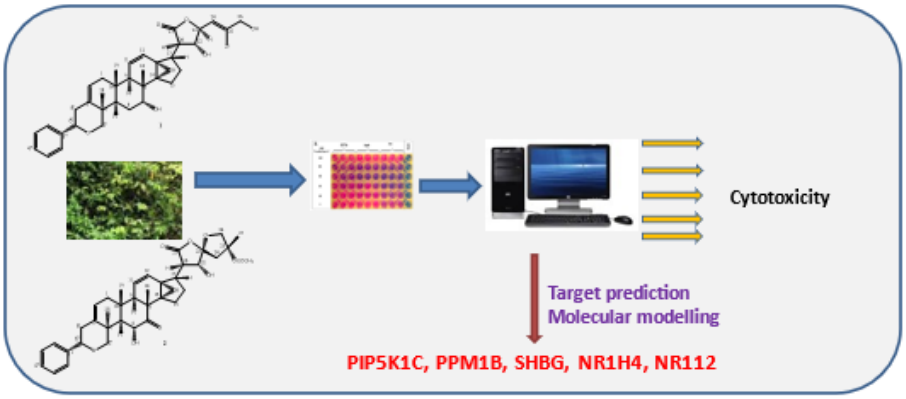

Figure 1: Summary of experimental setup

References:
[1] D. Osei-Safo, M. A. Chama, I. Addae-Mensah, *et al*. *Phytochem Lett*, **2008**, *1*, 147–150.
[2] C. Long, Y. Aussagues, N. Molinier, *et al*. *Phytochemistry*, **2013**, *94*, 184–191.
[3] S. X. Jing, S. H. Luo, C. H. Li, *et al*. *J Nat Prod*, **2014**, *77*, 882–893.
[4] L. H. Mervin, K. C. Bulusu, L. Kalash, *et al*. *Bioinformatics*, **2018**, *34*, 72–79.

OP04: Molecular Insight into the Interaction between the Spike Protein of the Wildtype, Delta and Omicron SARS-CoV-2 and the Human Angiotensin Converting Enzyme 2 (hACE2): Potential for the Design of Fusion Inhibitors

Samuel A Egieyeh[1*] and Alan Christoffels [2]

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[*]Corresponding author (Email: segieyeh@uwc.ac.za)

Background: The continuous mutation of the SARS-CoV-2, particularly at its spike protein, has been associated with increased transmissibility and of escape from neutralization by the immune system [1]. In this study we set out to gain insight into the interactions of the mutated receptor binding domain of the spike protein with hACE2. We hoped to provide an explanation for the reported increased transmissibility and also design peptides or small molecules that might inhibit or reduce the interaction of the mutant and wild type spike protein with the hACE2 receptor.

Methods: A combination of three-dimensional protein model characterization, protein-protein docking, molecular docking, and molecular dynamics were used to identify potential differences in the electronic potential distribution, solvation energy, interaction energy, interacting residues, and dynamics of the mutants (Delta and Omicron) and wild type spike proteins. Pharmacophore modeling was used to predict potential fusion inhibitors.

Results: Using the methods stated above, we observed differences in the protein properties, electronic potential distribution, solvation energy, interaction energy, interacting residues, and dynamics between the mutants (Delta and Omicron) and wild type spike proteins. Potential fusion inhibitors were identified by pharmacophore modelling of the receptor binding motif of the spike proteins.

Conclusion: The study showed differences in the receptor binding motif of the mutants (Delta and Omicron) and wild type spike proteins which can be exploited to design potential fusion/entry inhibitors.

Keywords: delta, fusion, inhibitors, omicron, spike proteins, SARS-CoV-2, wildtype

References:

[1] C. Rees-Spear, *et al*. The effect of spike mutations on SARS-CoV-2 neutralization. *Cell Reports*, **2021**, *34*, 108890. doi:10.1016/j.celrep.2021.108890

OP05: Cheminformatics Analysis of Ring Systems in Natural Products

Ya Chen,[1*] Cara Rosenkranz,[2] Steffen Hirte,[1] and Johannes Kirchmair[1]

[1]Department of Pharmaceutical Sciences, Division of Pharmaceutical Chemistry, Faculty of Life Sciences, University of Vienna, 1090 Vienna, Austria

[2]Center for Bioinformatics (ZBH), Universität Hamburg, 20146 Hamburg, Germany

[*]Corresponding author (Email: ya.chen@univie.ac.at)

Background: More than half of all modern small-molecule drugs are related, to some extent, to natural products (NPs) [1]. Ring systems form the structural core of many drugs and are often essential to bioactivity [2]. However, there is still limited understanding of NP ring systems and how they could be utilized to boost drug design and discovery.

Methods: We compiled comprehensive, curated data sets of NPs, synthetic compounds and approved drugs, from which we extracted the ring systems. Cheminformatics approaches were employed to analyse the structural and physicochemical properties of NP ring systems, and the coverage of NP ring systems by readily purchasable, synthetic compounds. In addition to common 2D physicochemical properties, such as molecular weight and the number of nitrogen/oxygen atoms, we also considered the 3D shape and electronic properties. Importantly, we deployed a new algorithm to maximize the use of the available stereochemical information on ring systems.

Results: This study shows the structural diversity of NP ring systems. Compared to the ring systems observed in synthetic compounds, those observed in NPs are more complex and more of them are macrocycles. Approximately one in two NP ring systems are represented by ring systems with identical or related 3D shape and electrostatic properties in synthetic compounds, but only about 2% of the ring systems observed in NPs are present in approved drugs.

Conclusion: The results presented in this work quantify and underline the diversity of NP ring systems and their importance to drug discovery. The study highlights and quantifies the huge potential of ring systems that are yet to be explored by chemists.

Keywords: cheminformatics; natural products; ring systems

References:

[1] D. J. Newman, G. M. Cragg. *J Nat Prod*, **2020**, *83*, 770–803.
[2] P. Ertl, *J Chem Inf Model*, **2021**, DOI:10.1021/acs.jcim.1c00761.

OP06: Ersilia, a Hub of Open-Source AI/ML Models for Drug Discovery and Global Health

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The Ersilia Open Source Initiative (EOSI; https://ersilia.io) is a non-profit organization with the mission to strengthen the research capacity in low- and middle-income countries. In particular, EOSI is focused on disseminating and deploying artificial intelligence and machine learning (AI/ML) tools for drug discovery as a means to minimize the cost and number of laboratory experiments. The main asset of EOSI is the Ersilia Model Hub, a free, online, open-source platform where scientists can browse through a catalogue of AI/ML models, select the ones that are relevant to their research and run predictions online. We gather, in a single resource, two classes of models. On the one hand, we collect models developed by third parties and available in scientific publications. On the other hand, we develop models in-house and in collaboration with research groups that operate in the so-called Global South. In this presentation, I will explain how the Ersilia Model Hub can be deployed in the form of a fully functional, comprehensive virtual screening cascade that is coupled with medicinal chemistry, parasitology and ADME experimental pipelines. I will put special emphasis on AI/ML models that can handle natural product(-like) compounds.

Keywords: automated machine learning; QSAR; natural products

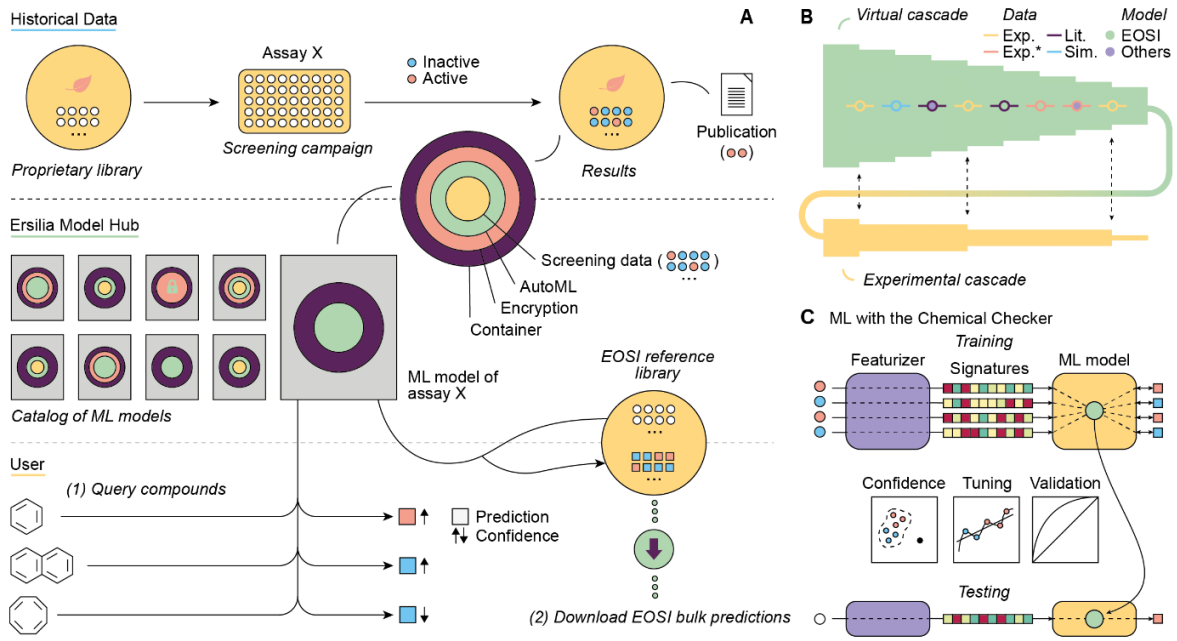

Figure 1: Scheme of the Ersilia Open Source virtual screening cascade.

OP07: A Taste of Nature – Predicting and Modulating Bitterness

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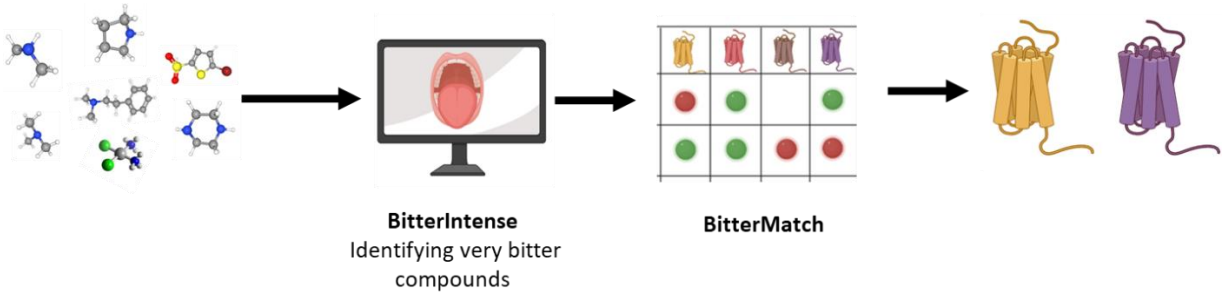
Bitter taste is innately aversive, and is often considered a sentinel of toxicity, helping to prevent the consumption of poisons. However, the bitterness-toxicity relation is not always pronounced [1] and many plant-derived molecules are bitter and healthy. Building upon the dataset of bitter molecules we are curating, the BitterDB [2], we developed Machine Learning tools that predict bitter [3] and intensely bitter [4] taste, based on the chemical features of the compounds.

Humans have 25 subtypes of bitter taste receptors of varying specificity [5]. We developed the BitterMatch algorithm which predicts associations of ligands with bitter taste receptors with ~80% precision at ~50% recall.

Together, these tools provide an in-silico pipeline, as will be illustrated for sets of molecules, including polyphenols. Discovery of bitter taste antagonists will be discussed as well.

Our results highlight the importance of integrating experimental data into computational analysis, help unravel structural aspects of molecular recognition, and provide a framework for iterative discovery of taste activity of natural compounds.

Keywords: BitterDB; bitterness; taste prediction.



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OP07-2: Evaluation of Trypanocidal Activity and Mode of Action of a Steriod from *Vitex simplicifolia* Leaves

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Background: Trypanosomiasis is a disease of major importance in both human and animals and has continued to threaten health and economic development [1]. Current therapeutic agents for the disease are laced with resistance and toxicity issues which calls for better options. Since plants have proven to be worthy source of effective and safe drugs and drug-leads, we turn to them here.
Methods: The leaves of *V. simplicifolia* were collected, identified, extracted with methanol, and fractionated using dichloromethane (DCM) following the procedures as described in our earlier work [2]. We followed combined vacuum liquid chromatography (VLC) using silica gel (230-400 mesh, 30 x 30 cm, 500 g) as the stationary phase and semi-preparative HPLC (Dionex P580) system coupled to photodiode array detector (UVD340S) to isolate, purify and characterize the obtained phytochemical. The plant fraction and compound were assayed against *Trypanosoma brucei rhodesiense* (STIB 900), *T. cruzi* blood stream forms and L6 cells. We employed Swiss Target Prediction and GeneCard databases to retrieve drug targets for the isolate and the two pathogens and used the Draw Venn Diagram platform analysis to identify the common targets of both the disease and the isolate. Lastly, bioinformatics tools and techniques were applied to predict biological target(s) of the isolate.
Results: Methanol leaf extract of *V. simplicifolia* moderate trypanocidal activity against *T. b. rhodesiense* (IC_{50} = 14.2 µg/ml). The DCMF brought 56.25 % reduction in parasitaemia at 100 mg/kg in *T. b. brucei* infected mice. Further chromatographic separation of DCMF with gradient of DCM : methanol yielded a steriod identified as ajugasterone C. The isolate was effective against *T. b. rhodesiense* (IC_{50} = 10.12 ± 0.3) and *T. cruzi* (IC_{50} = 46.05±1.5), however, it impact on the mammalian skeletal myoblast cell line (L6 cells) raises toxic concern (IC_{50} > 100 µg/ml) (SIT.b.r > 9.80 and SI *T.cruzi* > 2.01). Through bioinformatics manipulations we found the isolate interacts with *Trypanosoma* cysteine cathepsins (CatL and CatB) to exhibit their activity. Also, interaction with adenosine kinase (ADK) was identified with regards to T. b. rhodesiense. These mechanism of action are valuable in optimization exercises.
Conclusion: Plant and plant products have again proven useful in drug development against trypanosomal infections. Although phytochemicals are known to have high safety profile, our isolate raised toxicity concern. Mechanism of action of the compounds identified by computer predictions will be of help in modifying the compound to improve efficiency and safety.
Keywords: bioinformactics tools; binding mode; tryanosomal activity; *Vitex simplicifolia*.

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OP08: *In Silico* Polypharmacology and Efficacy of Natural Products

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Computational methods employed in drug discovery have accelerated the processes of drug design, with more than 70 drug discovered using this approach are in market today. In this talk, I will first expose the participant into the concept of polypharmacology, where one natural product can have multiple targets. In the second part of my talk, I will focus on the efficacy of natural products in aqueous environment. I will give particular emphasis on the solubility and aggregation issue of drug molecules and how this relates to the efficacy of the natural products. Finally, I will discuss some success stories of chemo-bio informatics approaches in drug design.

Keywords: efficacy; *in silico*; natural products; polypharmacology.

OP09: Insights into Intramolecular Interactions of Transition Metal-Bis-(*N*-Heterocyclic Carbene) Complexes and Topological Unraveling the C–H Bond Activation from QTAIM/ELF/EDA/NBO and BET Theory

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A new class of *N*-heterocyclic biscarbene ligands (BisNHC) ligands has been developed. These new ligands were installed on to transition metals generating bis *N*-heterocyclic carbene transition metal complexes of C2v symmetry. However, this project describes the bond properties and electronic structure of novel tetrahedral and square planar CH2-bridged bis-(*N*-heterocyclic carbene) transition metals halides. Figure 1 highlights the molecular building adopted and three **C∩C** coordination modes [(a), (b) and (c)] have been considered. In this figure, **X** refers to halide (Cl, Br and I) involved and **M** designates the divalent metal cations (Ni^{2+}, Pd^{2+} and Pt^{2+}).

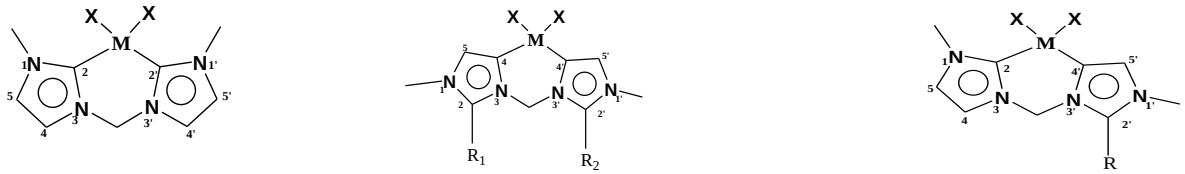

Figure 1: Numbering system of the bis-*N*-heterocyclic carbene complexes

Some of these complexes facilitate very favorably as catalysts for the oxidative activation of the C–H bonds of hydrocarbons. In a context where natural gas, mainly lower alkanes (methane 60%, propane 5% and LPG) constitute a huge resource of fossil fuels and feedstocks in the worldwide, the design and implementation of such compounds on the direct oxidation of alkanes is worthy [1]. These types of complexes are widely used in the catalytic petrochemical conversion of lower alkane into alcohol because of their more stable metal-ligand bond. It is important to note that metal-halide bonds play a decisive role in these reactions. These factors can be fine-tuned to achieve better catalytic activity. We aimed to propose oxidative activation reaction mechanisms for these complexes to facilitate their synthesis.

Reference:

[1] D. Munz and T. Strassner, *Angewandte Chemie International Edition*, **2014**, *53*, 2485-2488.

OP10: Trigonelline: A Promising Compound for The Treatment of Alzheimer's Disease

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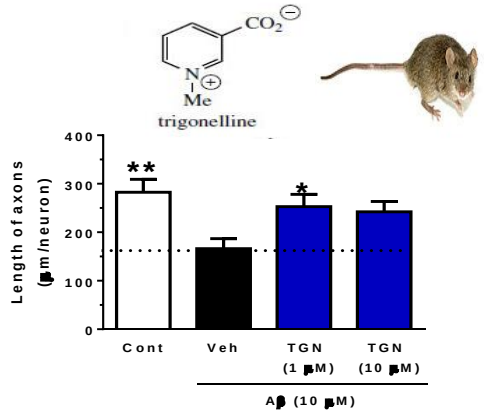
Trigonelline is a major alkaloid component derived from *Trigonella foenum-graecum* L. (fenugreek) and has been reported before as a potential neuroprotective agent, especially in Alzheimer's disease (AD). However, the previous data were unclear and used model mice were not well established. In the present study, the effect of trigonelline on memory function was investigated in Alzheimer's disease transgenic model mouse, 5XFAD which overexpresses mutated APP and PS1 genes [1,2]. Oral administration of trigonelline for 14 days significantly enhanced object recognition and object location memories. Plasma and cerebral cortex were isolated at 30 min, 1h, 3h and 6 h after oral administration of trigonelline. LC-MS/MS analysis indicated that trigonelline was detected in both of plasma and cortex from 30 min after, suggesting good penetration of trigonelline into the brain. In addition, trigonelline significantly ameliorated axonal and dendrite atrophy in Amyloid β-treated cortical neurons. Analysis of target proteins of TGN in neurons by a drug affinity responsive target stability (DARTS) method identified that creatine kinase B-type (CKB) is a direct binding protein of TGN. Treatment with a CKB inhibitor cancelled the TGN-induced axonal and dendritic growth. These results suggest that trigonelline could be a promising therapeutic candidate for AD.

Keywords: Alzheimer's disease; cortical neurons; LC-MS/MS analysis; *Trigonella foenum-graecum ;* trigonelline.



References:

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OP11: Search for Schweinfurthins and other Secondary Metabolites from *Macaranga Occidentalis* (Euphorbiaceae) and Evaluation of Possible Anticancer Activity

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Background: A new class of prenylated stilbenes called Schweinfurthins A-D, exhibiting promising anti-cancer activities as reported by the U.S National Cancer Institute (NCI) were first isolated from the Cameroonian medicinal plant *Macaranga schweinfurthii* (Euphorbiaceae). Schweinfurthins E-H were later isolated from *M. alnifolia* and recently, K-Q were isolated from *M. tanarius*. [1-3] These interesting results prompted the investigation of other Cameroonian *Macaranga* species to isolate the Schweinfurthins and other lead compounds that could be developed as viable anticancer agents.
Methods: *M. occidentalis* stem bark was collected from Likombe village at the foot of Mount Cameroon, South-West region of Cameroon, and was subjected to phytochemical investigation. Six compounds were isolated, labelled MOC1-MOC6 which were then analyzed using GC-MS and ^{1}H-NMR analysis.
Results: Of three of the compounds notably MOC1-MOC3 have revealed them to be a mixture of 9,12-Octadecadienoic acid-(*Z*,*Z*)-methyl ester (Methyl linoleate) and 9-Octadecenoic acid-E-methyl ester (Methyl-E-oleate) (MOC1), a mixture of phytosterols ß-Sitosterol acetate, γ-Sitosterol, ß-Stigmasterol and Campesterol (MOC2) and a pentacyclic triterpenoid 28-Norolean-17-en-3-ol (MOC3).
*Conclusion***:** While none of the compounds falls in the class of Schweinfurthins, GC-MS and spectroscopic analysis are currently ongoing to determine the structures of the other isolated compounds (MOC4-MOC6), together with the unidentified compounds on the GC-MS chromatogram (RT:17.847, RT:20.142 and RT:27.967) and their subsequent submission for anti-cancer screening.
Keywords: Euphorbiaceae; *Macaranga occidentalis*; 28-norolean-17-en-3-ol; Schweinfurthins

References:
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OP12: Molecular Docking and In Silico ADMET Predictions of Amodiaquine Derivatives as Antimalarial Agents.

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Background: Malaria is a life-threatening disease responsible for half million deaths annually, and with nearly half of the world's population at risk. The rapid drop in observed cases of malaria in the last two decades has been due to a combination of preventive and therapeutic remedies. However, the development of new drugs is critical because of the diminished effectiveness of current antimalarial agents mainly due to parasitic resistance, side effects and cost.

Methods: In this study, the *in-silico* absorption, distribution, metabolism, excretion and toxicity (ADMET) study of some substituted amodiaquine compounds as well as predict the potential interaction modes and binding affinities of the designed ligands with the enzymes of different pathways (folate and glycolytic) is explored.

Results: Molecular docking was used to explore structural motifs responsible for the interactions between triose phosphate isomerase (TPI), glyceraldehyde-3-phosphate dehydrogenase (GAPDH) and dihydrofolate reductase (DHFR) from human and *Plasmodium* cells with 10 novel amodiaquine derivatives. All the ligands modeled, interact with all three enzymes. Human and *Plasmodium falciparum* TPI bind with amodiaquine derivatives using two distinct binding sites and residues. Also, the top-scoring ligand AmoJ shows a high binding affinity with all the receptors compared to amodiaquine and other derivatives.

Conclusion: This ligand can thus serve as pharmacophore for the development of novel antimalarial drugs.

Keywords: Malaria, *Plasmodium falciparum*, antimalarial activity, molecular docking, 4-aminoquinoline drugs, ADMET study, binding affinity.

OP13: A Molecular Investigation of the Solvent Influence On Inter- and Intra-Molecular Hydrogen Bond Interaction of Linamarin

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Linamarin has been reported to have anticancer activities; however, its extraction and isolation using different solvents yield a low amount. Therefore, understanding the physical properties, such as solvents' solubility, membrane permeability and lipophilicity and how they are associated with different solvents, is a paramount topic for discussion, especially for its potential as a drug. Linamarin has a sugar moiety with many polar groups responsible for its physical properties. Following current trends, a molecular dynamics simulation is performed to investigate its physical properties and how different solvents, such as water, methanol (MeOH), dimethyl sulfoxide (DMSO) and dichloromethane (DCM), affect such properties. In this work, we have investigated the influence of intermolecular and intramolecular hydrogen bonding and the influence of polar and nonpolar solvents on the physical properties of linamarin. Furthermore, solvation free-energy and electronic structure analysis are performed. A detailed analysis shows intermolecular hydrogen bonding between polar solvents (water, MeOH and DMSO) and the hydroxyl oxygens of linamarin. Water exhibits the strongest interaction with linamarin's functional groups among the investigated solvents. The solvation free energy calculations confirm DMSO to be the best solvent since it prefers to interact with linamarin over itself, while water prefers to interact with itself. The solute–solvent interactions are strongest between linamarin and DMSO, the solvent–solvent interactions are strongest in water. As a result, the solvation free-energy calculations reveal that linamarin solvation is most favorable in DMSO.

OP14: Hepatoprotective Effects of Extracts, Fractions and Compounds from *Pentaclethra macrophylla* Benth against Experimental Hepatotoxic Models

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Pentaclethra macrophylla Benth (Mimosaceae) is a medicinal plant commonly used in Cameroon to treat several diseases such as itching and liver diseases. Lipid peroxidation is an important process in the development of many diseases, especially hepatotoxicity-driving liver diseases. The aim of this study was to isolate secondary metabolites responsible for the hepatoprotective effect of the ethanol extract of *Pentaclethra macrophylla* stem bark and to study their structure-activity relationship. We used hydrogen peroxide (H_2O_2)-induced lipid peroxidation to hepatocyte membranes' model to successively assess the hepatoprotective-bioguided-fractionation of the ethanolic extract of *P. macrophylla*. For the *in vivo* hepatoprotective test, mice were treated orally with the ethyl acetate (EtOAc) fraction of the ethanol extract and subjected to D-galactosamine/lipopolysaccharide-induced (GaIN/LPS) hepatotoxicity. Blood samples were collected for alanine aminotransferase (ALAT), aspartate aminotransferase (ASAT), TNF-α and IL-1β assays. The ethanol extract was suspended in distilled water and successively extracted with EtOAc and *n*-BuOH to yield the EtOAc and *n*-BuOH fractions as well as the residual aqueous fraction. The hepatoprotective test showed that the EtOAc fraction was the most effective (IC_{50}: 3.214 µg/mL) compared to silymarin used as reference (IC_{50}: 117.4 µg/mL). Its fractionation by column chromatography yielded three active sub-fractions which were purified to give one monoglyceride, one carboxylic acid, two steroids, two tannins and one terpenoid. Their structures were established based on their mass spectrometry, 1D and 2D NMR data and by comparison of their data with those of related compounds present in the literature. Compound 11-*O*-galloyl bergenin (IC_{50}:1.8 µg/mL) was the most effective. *In vivo*, the EtOAc fraction significantly reduced the serum level of ALAT, ASAT and TNF-α, and increased the liver protein content. Thus, this fraction could further be submitted for more investigations as lead for liver diseases.

Keywords: bioguided-fractionation; GaIN/LPS; hepatoprotective-activity; lipid-peroxidation; *Pentaclethra macrophylla*; structure-activity-relationship.

HS01: Genome Mining using antiSMASH, and the antiSMASH and MIBiG databases

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With the increased availability of genome data, software tools to search for interesting biosynthetic gene clusters (BGCs) have gained in popularity as a method for discovering specialized/secondary metabolites. Initially released in 2011, the "antibiotics and Secondary Metabolites Analysis Shell (antiSMASH)" [1] has established itself as the gold standard software for microbial genome mining. To put antiSMASH predictions into context, the antiSMASH database [2] contains almost 150,000 predicted BGCs from over 25,000 bacteria, archaea, and fungi. While the antiSMASH database contains many predicted clusters, the Minimum Information about a Biosynthetic Gene cluster (MIBiG) database [3] contains around 2,000 manually curated BGCs backed by literature, the most comprehensive collection of known BGCs.

In this hands-on session, participants will learn some background on how antiSMASH predicts BGCs. They will then gain some experience in running antiSMASH and interpreting the results of such runs. Participants will then learn how to use the antiSMASH and MIBiG databases to gain additional insights into the predicted BGCs.

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[3] S.A. Kautsar, K. Blin, et al. *Nucl. Acids Res.*, **2020**, *48(D1)*, D454-D458

HS02: Building a Machine Learning-Based Bioactivity Predictor

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In this session, you will learn how to build your own machine learning-based tools to classify and predict the biological activities of small molecules. You will also learn how to build machine learning-based virtual screening tools to rapidly search millions of molecules. The skills learned can be applied to other areas with different data as well. A common step in drug discovery is to identify compounds that are active against a biological target. Computational models are often used to predict the activity and further prioritize the compounds for experimental testing. In this regard, a routine task is to sample a fraction of the drug-like compounds available in the chemical databases. It is often warranted to sample the highest fraction of the drug-like compounds available which is estimated to be the size of greater than ten to the power sixty-three. Even with routinely available methods such as molecular docking and computational resources available to scientists around the world, the screening of only a small fraction of molecules could be possible so far. Machine learning and deep learning-based applications have received a significant boost in performance and are thus being adopted significantly for this task. This project demonstrates how to build such machine learning models to rapidly search millions (or possibly billions) of molecules. What you will learn include how to install software packages; how to collect bioactivity data; how to process bioactivity data; how to process chemical structures; how to carry out molecular feature engineering; how to build, train and evaluate bioactivity classification models; how to prepare virtual a screening dataset; how to conduct machine learning-based virtual screening; and how to select chemical hits.

HS03: Visualization of RNA-Seq with Galaxy Framework

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Background: Heatmaps are commonly used for visualizing the differentially expressed genes in the samples [1]. The current galaxy training tutorial examines the expression profiles of basal and luminal cells in the mammary gland of virgin, pregnant and lactating mice [2] using the *heatmap2* tool available in the Galaxy.

Methods: Initially the dataset including the normalized counts file, differentially expressed (DE) results file and genes of interest are imported into the Galaxy history. Further, the top significant genes are extracted from the DE results file that passes the threshold, followed by the extraction of the normalized counts for the top genes. Finally, the heatmap is generated from these datasets.

Results: A heatmap will be generated in which the top genes differentially expressed in the luminal cells from the pregnant mice versus the luminal cells from the lactating mice will be plotted.

Conclusion: Heatmaps generated from the heatmap2 tool in the Galaxy are used to visualize the differential expression of genes in RNA-Seq samples. This concludes the tutorial additionally the steps can be used to generate a sharable Galaxy workflow.

Keywords: Galaxy; heatmap; RNA-Seq

References:
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HS04: Virtual Screening for the Fast and Cheap Identification of Bioactive Natural Products

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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 IV: Speakers

Jude Betow

Jude Betow is a Ph.D. student in Chemistry at the University of Buea, Cameroon, and a part-time lecturer at the Strategic University Institute of the Estuary (IUEs/INSAM), Douala, Cameroon. He obtained his B.Sc. in Chemistry with a minor in Pharmaceutical Chemistry; and an M.Sc. in Chemistry at the same university. He is a junior researcher in organic synthesis and natural product chemistry, with a research focus on the discovery of bioactive novel molecules mainly from medicinal plants. The biological activities of interest include antimicrobial, antiproliferative, and activities against neglected Tropical diseases. He has also included molecular modeling and computational techniques to suggest the mode of action of lead compounds in drug discovery studies. He also has experience in various plant extraction methods, chromatography techniques, isolation, and characterization of plant components.

Özlem Taştan Bishop

Özlem is full professor in structural bioinformatics at Rhodes University. She received her BSc degree in Physics from Boğaziçi University, Istanbul, Turkey. Then she moved to the Department of Molecular Biology and Genetics at the same University for her MSc degree. She obtained her PhD from Max-Planck Institute for Molecular Genetics and Free University, Berlin, Germany in 2003. While doing her PhD, Özlem became interested in structural biology, and during her postdoctoral positions (Texas University, USA; University of Western Cape and University of Pretoria, South Africa) she gained experience in structural bioinformatics as well as structural biology. In 2009, Özlem took up an academic position at Rhodes University, South Africa. She established Research Unit in Bioinformatics (RUBi) in 2013. She has graduated 16 PhD and over 30 MSc students since she joined Rhodes University. Özlem's broad research interest is structural bioinformatics and its applications to drug design and development. Her recent interest is in the allosteric mechanisms of proteins and understanding the effects of nonsynonymous single nucleotide variations on protein structure and function, in order: to decode the underlying causes of many inherited diseases; to uncover drug resistance mechanisms; and to investigate drug sensitivity issues in certain populations for precision medicine purposes. She has published over 80 research articles.

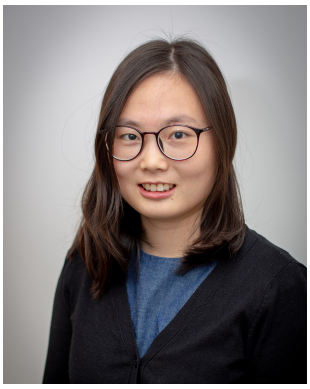
Kai Blin

After obtaining a degree in bioinformatics from the computer science faculty at the University of Tübingen in 2009, Kai switched to Institute for Microbiology and Infection Medicine at the same university to obtain his PhD. During his PhD project, he co-developed the antiSMASH genome mining tool, initially released in 2011 and currently the most popular tool in the field with ~ 1,200,000 jobs and ~ 7500 citations. Building on his software engineering knowledge obtained working on Open Source software projects since his undergrad days, Kai has focused on developing translational bioinformatics tools and databases. After a postdoc at the Max Planck Institute for Biology of Ageing in Cologne, Kai returned to natural products research and joined the Novo Nordisk Foundation Center for Biosustainability (NNFCFB) at the Technical University of Denmark, in Lyngby, Denmark. He is currently working as a Senior Researcher in the Natural Product Genome Mining section run by Tilmann Weber where he heads the bioinformatics group. As a certified Software Carpentry instructor since 2016, Kai is happy to pass on his knowledge about software development in the life sciences and genome mining and has regularly taught courses on these subjects.

Mary Anti Chama

Dr. Mary Chama is a Senior Lecturer at the University of Ghana. She is a natural product chemist with a research focus in the discovery of bioactive novel molecules mainly from medicinal plants. The biological activities of interest include antimicrobial, antiproliferative, cytotoxicity and activity against neglected tropical diseases. She has included computational target prediction, and molecular modelling to suggest mode of action in the drug discovery studies. Has experience in various plant extraction methods, chromatography techniques, isolation and characterization of plant component.

Ya Chen



Dr. Ya Chen (Anya) is a postdoctoral researcher in the Computational Drug Discovery and Design Group (COMP3D) of the Department of Pharmaceutical sciences, University of Vienna, Austria. She specializes in the development and application of in silico methods for natural products research. In 2013, she earned her Bachelor's Degree in Pharmacy at Jilin University, China. She then studied Medicinal Chemistry at Peking University and earned her Master's Degree of Science in 2016. In 2020, she was awarded a PhD in cheminformatics from Universität Hamburg, Germany.

Lucie Karelle Djogang

https://www.researchgate.net/profile/Djogang-Karelle

Lucie is a PhD student in the Computational Chemistry Group, under Prof. Alphonse Emadak at the University of Yaounde I (Cameroon). She completed a Master of Science in Coordination Chemistry at the University of Yaounde I in the group of Prof. Justin Nenwa where she synthesized an organic-inorganic complexes in aqueous-ethanol middle. She then changed research areas from coordination chemistry to theoretical chemistry especially molecular modeling with a focus on predicting potential antimalarial drugs through molecular docking. In 2020, she got Eugen-Ionescu scholarship at the University of Alexandru Ioan Cuza, Iasi; Romania under the supervision of Prof. Ionel Humelnicu (Theoretical Chemistry Group). She is also a member of Organization for Women in Science for the Developing-Cameroon (OWSD-CAM) National Chapter.

Pieter Dorrestein

Dr. Dorrestein is Professor at the Skaggs School of Pharmacy and Pharmaceutical Sciences, and departments of Pharmacology and Pediatrics, University of California - San Diego. He is the Director of the Collaborative Mass Spectrometry Innovation Center and a Co-Director, Institute for Metabolomics Medicine in the Skaggs School of Pharmacy & Pharmaceutical Sciences, and Department of Pharmacology. Since his arrival to UCSD in 2006, Dr. Dorrestein has been pioneering the development of mass spectrometry methods to study the chemical ecological crosstalk between population of microorganisms, including host interactions for agricultural, diagnostic and therapeutic applications. He is the advisor to Cybele and is a co-founder and scientific advisor for Ometa and Enveda.

Miquel Duran-Frigola

Miquel Duran-Frigola, PhD

Lead Scientist and Co-Founder at Ersilia Open Source Initiative

Email: miquel@ersilia.io

Twitter: @mduranfrigola

Miquel's research interests lay at the intersection between drug discovery and large-scale biological data analysis. During his PhD studies and early career, Miquel developed several in silico methods, producing scientific publications in a broad range of topics, from theoretical chemistry to cell-based data analysis. Along this process, he has worked at IRB Barcelona, the Massachusetts Institute of Technology (MIT), Tel Aviv University, ISGlobal-CISM (Mozambique), CIDRZ (Zambia) and H3D (South Africa). Currently, Miquel is Lead Scientist at the Ersilia Open Source Initiative. With Ersilia, he hopes to apply his data science skills in underfunded settings such as research institutes in Low and Middle Income Countries.

Samuel Ayodele Egieyeh

Dr. Samuel Ayodele Egieyeh is a seasoned and highly experienced pharmacist (qualified in 1997) with Bachelors and Masters degrees in Pharmacy, and a Ph.D. in Bioinformatics. He also has a post-graduate diploma in clinical research and drug development from the University of Basel, Basel Switzerland. He is currently a senior lecturer at the discipline of Pharmacology and Clinical Pharmacy, School of Pharmacy, University of the Western Cape, Cape Town South Africa. He leads the Computational Pharmacology and Cheminformatics Group (CPCG). His research focuses on computational drug discovery and design; data science (including cheminformatics, bioinformatics, machine learning and biostatistics techniques) for predictive drug development and precision medicine for infectious and non-communicable diseases. His presentation will show the use of data science in drug discovery and development, therapeutics, and precision medicine. The presentation will also introduce the "University of the Western Cape's Computational Pharmacology and Chemoinformatic Platform" that is used to analyse hit compounds from high-throughput assays (HTS) available in public bioactivity databases. The platform provides data analytics and data mining tools for researchers in drug discovery and design to analyse and mine useful data from their in vitro experiments in order to make rational and viable drug discovery and design decisions.

Mai M. Farid

Dr. Mai Farid is an Assistant Professor in Phytochemistry and Plant Systematic Department, Pharmaceutical Industry Research Division, National Research Center, Cairo, Egypt. She is a natural product chemist with a research focus on the discovery of natural compounds from medicinal plants. She conducted research on the effect of natural medicine on Alzheimer's disease while she was a postdoctoral researcher in the Section of Neuromedical Science, Division of Bioscience, Institute of Natural Medicine, University of Toyama, Japan. she is a member of many scientific projects and Committees. She has experience in various plant extraction methods, isolation and characterization of natural compounds, chromatography techniques and biological activity of natural components on Alzheimer's disease.

Akachukwu Ibezim

Akachukwu Ibezim received his Ph.D. in Medicinal Chemistry in 2018 from the University of Nigeria, Nsukka under the co-supervision of Profs Ngozi Justina Nwodo and Chika John Mbah. His main research interest is in the application of computers in drug discovery. He started his journey into the world of computer-aided drug design in the Chemical and Bioactivity Information Center, University of Buea, Cameroun in 2014 under Fidele Ntie-Kang. During his short stay in the University of California, San Diego in the lab of Prof. Jair L. Siqueira-Neto he worked on using computers to identify trypanosomal cysteine proteases inhibitors and phenotypic cell-based screening to confirm activity anti-trypanosomal activity of small molecules of both natural and synthetic origin. Dr. Ibezim is currently in the lab of Prof. K. Ramanathan, Vellore Institute of Technology, India for his post-doctoral fellowship under TWAS funding.

Dušanka Janežič

Dušanka Janežič is Full Professor at the Faculty of Mathematics, Natural Sciences and Information Technologies at the University of Primorska (Slovenia). Founder of molecular modeling research in Slovenia with her research group currently ranking as one of the top research group in the field wordwide. Has published 2 scientific books and 130 publications in SCI journals with over 3000 pure citations in Web of Science database, and h-index 23. One of the Editors in the ACS Journal of Chemical Information and Modeling (2001-2014). In 2013, Recipient of Žiga Zois Award for outstanding research achievements in mathematics in natural sciences. In 1999, Recipient of Ambassador in Science of the Republic of Slovenia Award. From 2013-2019 she was appointed by the government of Republic of Slovenia as council member of the National Agency of Qualitative Evaluation of Higher Education in Slovenia. She worked in the USA as a visiting researcher at the National Institute of Standards and Technology. As a Senior Fulbright Scholar she conducted research in the USA at the National Institutes of Health. She worked at the Technical University of Munich, Germany as a DAAD fellow. Her current research interests include graph theory development, prediction of protein-protein and protein-ligand binding sites, biomolecular simulations, and the application of these techniques to problems in pharmaceutical research and drug development.

Darshana Joshi

Darshana Joshi is currently pursuing her Master's course in Bioinformatics at Guru Nanak Khalsa College of Arts, Science and Commerce from Mumbai University, India. She is a Member of Tarunavadaanenasaha Muktbharatonnayana Samstha (TMS) since May 2021.

Jutta Ludwig-Müller

Prof. Jutta Ludwig-Müller is one of the organizers of the online workshop "Computational Applications in Secondary Metabolite Discovery (CAiSMD)". From 1999, she has been a Professor of Plant Physiology at the Technical University Dresden (Germany). After studying Biology at Frankfurt (Main) leading to a Diploma thesis on the topic "Auxin biosynthesis in Brassicaceae" (1981-1986), she completed her PhD dissertation in 1990 at the Botanical Institute of the Johann Wolfgang Goethe Universität (JWGU) in Frankfurt (Main) on the topic "Auxin biosynthesis and the role of auxins during the clubroot disease", with several visits to the laboratory of Dr. Ephraim Epstein, Volcani Center, Israel. After a research assistanship and postdoctoral stay in the USA, she completed her Habilitation in 1996. From 1995 to1999, she was an Assistant Professor at the Botanical Institute of the JWGU. During this period she made several visits to the laboratory of Dr. Jerry D. Cohen, United States Department of Agriculture, Beltsville, Maryland (USA). Her research focuses on mechanisms leading to plant-pathogen (clubroot disease) interactions or the interaction with beneficial microorganisms (fungal endophytes). Her group is interested in the role of plant hormones and secondary plant products for development of pathogenic or symbiotic interactions of fungi with host plants. For better understanding of the events leading to pathogenesis, the team have begun to identify differentially expressed genes during host/pathogen interaction. She is also interested in the role of auxins and glucosinolates during plant development and therefore they study the biosynthesis, metabolism and regulation mechanisms controlling the endogenous concentrations of these compounds. In addition to glucosinolates, her team also investigates the bioactivity of other secondary plant metabolites such as flavonoids and phenylpropanoids. In 2019, she was awarded the Spiridion Brusina Medal of the Croatian Society of Natural Sciences. She is a member of several scientific organizations, including the American Society of Plant Biology (ASPB) and the German Botanical Society (DBG) and Editor-in-Chief of the journal Journal of Plant Growth Regulation (Springer).

José L. Medina-Franco

Dr. Medina-Franco holds a BSc in Chemistry (1998, National Autonomous University of Mexico (UNAM), a MSc and Ph.D. degree (2005, both from the UNAM). In 2005, Dr. Medina Franco joined the University of Arizona as a postdoctoral fellow under the supervision of Prof. Gerald Maggiora and he was named Assistant Member at the Torrey Pines Institute for Molecular Studies in Florida in August 2007. In 2013, he conducted research at the Mayo Clinic. In 2014 he joined UNAM and now is Full Time Research Professor. He leads the DIFACQUIM research group at UNAM. The research focus is on chemoinformatics and computer-aided drug design with applications on epigenetic targets and natural products. Dr. Medina-Franco is member of the National Researcher System, National Council of Science and Technology in Mexico with the highest level, III. In 2017 he was named Fellow of the Royal Society of Chemistry (UK) and was Visiting Professor of the University of Montreal at Quebec in 2019. Dr. Medina Franco has published 250 peer-reviewed papers, 24 books chapters and issue one international patent. He has edited the books *Epi-Informatics* and *Food Informatics*. He serves as Chief Editor of the section "*In Silico Modeling and Artificial Intelligence*" of *Frontiers in Drug Discovery*; member of the Editorial Board of *Journal of Chemical Information and Modeling* and Lead Advisor of *F1000Research*, *Chemical Information Science*. He is member of the Scientific Advisory Board of the company Epigenavir, LLC (USA). Since 2007 he has been PI in several research grants. Dr. Medina Franco has supervised the research of over 30 postdoctoral fellows, Graduate and Undergraduate students. Research Group website (https://www.difacquim.com/).

Pankaj Mishra

Dr. Pankaj Mishra specializes in molecular artificial intelligence and computer-aided drug design. He holds a Doctor of Philosophy degree in natural sciences (magna cum laude) from the University of Freiburg, Germany under the supervision of Prof. Dr. Stefan Gunther, and a Master's degree in Pharmaceutical Chemistry from the Indian Institute of Technology. His Ph.D. research project was focused on developing one artificial intelligence algorithm for drug discovery. Here you can read about my work: https://freidok.uni-freiburg.de/data/218570. After a short postdoc at the same University, he launched a research education company (Uresearcher: https://uresearcher.com/) Uresearcher is now an 11 members team working from 4 time zones.

Thommas Mutemi Musyoka

Dr. Thommas Mutemi Musyoka has a Ph.D. in bioinformatics from Rhodes University, South Africa. He is involved in several computational studies for early stage identification of potential hits against infectious agents as well as deciphering their underlying mechanisms of drug resistance. He is also involved in the maintenance and upgrading of the South African Natural Compound Database (SANCDB). After a postdoctoral research fellowship in the Research Unit of Bioinformatics (RUBi), Rhodes University where he also mentored several postgraduate students working on different computational studies, he recently took up an academic position at Department of Biochemistry, Microbiology and Biotechnology, Kenyatta University, Nairobi, Kenya.

Masha Niv

Masha Niv is a Full Professor at The Hebrew University of Jerusalem, where she has been working for 14 years. She obtained her Bachelor of Science (B.Sc.) degree in Chemistry (cum laude) from the Hebrew University of Jerusalem (1989 - 1993), followed by a direct Ph.D. in theoretical chemistry from the University of Jerusalem (1994 - 2001). She carried out postdoctoral research at the Weill Cornell Medical College before moving back to the Hebrew University of Jerusalem to open her lab. She previously served as Vice Dean for Research, The Faculty of Agriculture, Food and Environment, promoting collaborative and international research. She is currently a Board Member Israel of the Institute for Advanced Studies (Jerusalem, Israel). Masha is a highly recognized scientist and a well-traveled conference speaker. Her research has been focused on the rational design of tastants, taste modulators, and drugs. Her group studies bitter and sweet molecules and their receptors, using in-silico, in-vitro and psychophysics tools.

Fidele Ntie-Kang

Fidele Ntie-Kang is one of the organizers of the online workshop "Computational Applications in Secondary Metabolite Discovery (CAiSMD)". He currently heads the Molecular Simulations Laboratory, Chemistry Department, University of Buea (Cameroon). He studied Chemistry at the University of Douala (Cameroon) from 1999 to 2004, leading to Bachelor's and Master's degrees. His Ph.D. was based on molecular modeling of anti-tubercular drug target to design novel inhibitors, followed by an Habilitation in Pharmaceutical Chemistry from Martin-Luther University Halle-Wittenberg, Halle (Saale) (Germany), under Prof. Wolfgang Sippl. He was formerly a Guest Professor or Lecturer at the Technical University, Dresden (Germany), is currently an Adjunct Professor at the Nelson-Mandela African Institution of Science and Technology, Arusha (Tanzania) and has been teaching a course on "Drug Design" in the Masters Program in Pharmaceutical Biology, University of Applied Sciences, Zittau/Görlitz (Germany). His current focus is the discovery of bioactive natural products from African flora by the use of virtual screening followed by in vitro assays. A major contribution of his research team has been the development of the African Natural Products Database (ANPDB). He has authored or co-authored more than 100 publications and has served as Associate Editor in several journals, as Guest Editor in special issues in the journals Molecules and Frontiers in Pharmacology. He holds several awards, including the Georg Forster Fellowship from the Alexander von Humboldt Foundation (Germany) and the Calistous Juma Fellowship from the Bill and Melinda Gates Foundation. He is a member of several academic societies, including the American Chemical Society and the Cameroon Academy of Young Scientists. He is the editor of the book series "Chemoinformatics of Natural Products" published by Degruyter.

Jean Moto Ongagna

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www.researchgate.net/profile/Jean-Moto-Ongagna

Jean Moto Ongagna defended his Ph.D. in physical and computational chemistry at the University of Douala, Cameroon under the co-direction of Prof. Luc Mbaze Meva'a and Prof. Desire Bikele Mama. He obtained his B.Sc. in Chemistry and an M.Sc. in Chemistry in physical chemistry from the same university. He is a postdoctoral researcher in theoretical coordination chemistry; especially molecular modeling. He has also included molecular modeling and computational techniques to suggest the reaction mechanism of activation and functionalization C-H bond of lower alkanes. In addition, he participated to the Virtual Conference on Chemistry and its Applications on Chemical Sciences for the New Decade.

Victor Chukwudi Osamor

Victor C. Osamor is a Full Professor of Computer Science, former HOD, Computer and Information Sciences and past Coordinator/ Director, Covenant University Center for Information Technology (CU CIT). Prof Osamor is also the Applied Research Coordinator for World bank - 6 million dollar funded Covenant Applied Information and Communication - African Center of Excellence (CApIC-ACE) research grant project with experience and previous involvement in NIH, NSF, H3Africa and H3Abionet research projects. He has experience in postgraduate supervision with graduated and current M.Sc and Ph.D students under his training. Prof Osamor is an Adjunct Professor and External Examiner to other Universities and a Grant Reviewer for Executive Government Agency of National Science Centre (Narodowe Centrum Nauki -NCN), Poland. His Ph.D is in Computer Science and Bioinformatics and Post-Doctorial fellowship is at University of Warsaw. He researches in Bioinformatics, Artificial Intelligence, Data analytics with other interest in Software techniques, Cyber security, Computer graphics and animation with certification in Artificial Intelligence, Predictive Analytics in IBM SPSS Modeller, Microsoft Technical Associate (MTA) in Database, Oracle Database and SQL programming. Prof Osamor is a Marie Curie Fellow and belongs to Marie Curie Alumini Association (MCAA), having experience in European Commission/EU Co-funded projects with European Research Center for Informatics and Mathematics (ERCIM). Prof Osamor is author of several books, co-editor of a textbook, reviewer and has several publications in reputable journal to his credit.

Lucas Paul

Lucas Paul is a PhD student at the Nelson Mandela African Institution of Science and Technology (NM-AIST), Tanzania under the African Development Bank (AfDB). He is also employed as an assistant lecturer at Dar es Salaam University College of Education (DUCE) under the Chemistry department. He obtained his master's in materials science and engineering at NM-AIST. His current Ph.D. research focuses on cyanogenic glycosides from cassava an African staple food, the main interest is to determine the structure of enzymes and how can be applied in the detoxification of cassava products. He has used computational modelling like homology modelling, molecular docking and molecular dynamics simulation to determine the structure of enzymes and understand the interaction mechanism with their substrate. He developed this research idea when he met Prof. Fidele Ntie-Kang in 2018 at NM-AIST during the Biophysics school.

Daniel Madulu Shadrack

Daniel Madulu Shadrack is a trained chemist, he holds a Ph.D. in Computational Biophysics. He works with the St John's University of Tanzania, Dodoma Tanzania. Daniel's research focuses on the use of computational methods such as molecular dynamics, metadynamics, free energy methods and molecular docking to understand biomolecular process towards drug design. Over the past five years, Daniel has acted the role as the Director and co-organizer of the Biophysics schools in Africa, of which the school has trained over 100 young scientists across the continent. Daniel has established several networks and research contacts across the world, the active network and collaborations are from Italy, Canada, South Africa, Kenya, Cameroon, Malawi and Ghana. Daniel is a Co-PI of three research projects, two projects in COVID-19 and one on malaria. Both projects involve the use of different computational and experimental techniques to identify small molecules as potential drugs.

Pierre Valery Kemdoum Sinda

Pierre Valery Kemdoum Sinda is a Ph.D. student at the Department of Chemistry< Faculty of Science, University of Dschang, Cameroon. He is affiliated to the research unit of applied and environmental chemistry. He obtained his Master's Degree with in Organic Chemistry / Natural Products Chemistry at University of Dschang. His current Ph.D. research focuses on study of the chemical constituents of two medicinal plants in Cameroon: *Helichrysum odoratissimun* (L.) Sweet (Asteracea) and *Pentaclethra macrophylla* Benth (Mimosaceae). The main interest is to determine bioactive compounds with antimicrobial and hepatoprotective activities in order to establish the structure-activity-relationship. He developed this research idea when he met Prof. Dr. Léon Azefack Tapondjou in 2018 during my thesis registration.

Kiran Kumar Telukunta

In 2018, Kiran completed his doctoral research in Pharmaceutical Bioinformatics at the University of Freiburg (Germany), while managing several Scientific IT infrastructure for Bioinformatic and Cheminformatics scientific projects, under Prof. Dr. Stefan Günther. Since then, he has worked on several projects, including as a Backend Developer and Software Engineer at Flowers-Software GmbH and Scientific Cloud Coordinator at VIB in Gent (Belgium). He has previously taught a course on ”Drug Design” in the Master’s Program in Pharmaceutical Biology, University of Applied Sciences, Zittau/Görlitz (Germany). He is Information System Administrator at ISES, a voluntary organisation in Freiburg (Germany). He is the one of the directors of the TMS Foundation, which voluntarily prepared the submission platform for this online workshop. During the workshop, he plans to present some general guidelines and underlying principles of gene cluster analysis with applications using Galaxy. He is currently working as a cloud architect for a renewable energy application.

Tilmann Weber

Tilmann Weber is a Professor for Natural Products Genome Mining and Associate Scientific Director of the "Natural Products Genome Mining Group" at the Novo Nordisk Foundation Center for Biosustainability of the Technical University of Denmark. His main research interest is focused on deciphering the molecular pathways and engineering the biosynthesis of natural products by combining genetic, biochemical and bioinformatics methods. He is a pioneer in developing software for the automated genome mining (CLUSEAN, antiSMASH, antiSMASH-DB) and analysis of secondary metabolite biosynthetic pathways. His group was able to firstly elucidate the biosynthetic pathways of the elfamycin family of antibiotics and is deeply involved in developing CRISPR-based metabolic engineering tools for actinomycetes. Tilmann Weber is a member of the Editorial Board of Scientific Reports, Metabolic Engineering, and Associate Editor for Synthetic and Systems Biotechnology.

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