PROGRAM & ABSTRACTS

THE FIFTH ASIA CONFERENCE ON PHARMACEUTICAL SCIENCES (ASIAPHARM V)

"Progress and Achievement in Pharmaceutical Sciences and Biomedicine"

Date: **AUGUST 16th-18th, 2023**

Venue: **TON DUC THANG UNIVERSITY, HO CHI MINH CITY, VIETNAM**

SPONSORS

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PREFACE

Asia Conference on Pharmaceutical Sciences (ASIAPHARM) is a traditional international conference dedicated to promoting advances in the field of pharmaceutical sciences. ASIAPHARM I was organized at Ton Duc Thang University, Vietnam, in 2016, and consequently, at Seoul National University (ASIAPHARM II, 2017), Bandung Institute of Technology, Indonesia (ASIAPHARM III, 2018), and Universiti Teknologi MARA, Malaysia (ASIAPHARM IV, 2019). During the Covid-19 pandemic, the conference was temporarily postponed. In 2023, the 5th Asian Conference on Pharmaceutical Science (ASIAPHARM V) will be resumed in Vietnam.

ASIAPHARM V will take place at the main campus of Ton Duc Thang University in Ho Chi Minh City, Vietnam, from August 16th to 18th, 2023. Being located near the populous and prosperous Mekong Delta, the vibrant Ho Chi Minh City, formerly known as Saigon, plays an important role in the history, geology as well as economy of the country. It is not only a commercial center but also a scientific, technological, industrial, and tourist center.

The theme of ASIAPHARM V is *"Progress and Achievement in Pharmaceutical Sciences and Biomedicine"*, which covers various areas, including organic and medicinal chemistry, pharmacology and clinical pharmacy, pharmaceutics and industry pharmacy, pharmacognosy, and natural products, pharmaceutical biotechnology, pharmaceutical management, and economics, pharmaceuticals analysis and quality control, multimodality drug development and others. The conference aims to exchange knowledge, address challenges, facilitate innovation, and promote cooperation in pharmaceutical sciences domestically and internationally.

The program of the Conference includes 120 reports, divided into nine scientific sessions and presented by prestigious authors from 11 countries of the world, comprising China, Indonesia, Japan, Korea, Malaysia, Myanmar, Taiwan (China), Thailand, The Philippines, USA, and Vietnam. There will be 8 plenary lectures, 60 oral presentations, and 50 posters during two days of the Conference. In addition, a special session for young scientists will be organized.

The Organizing Committee would like to express gratitude to Bepharco (Ben Tre Pharmaceutical JSC.), Suheung Co. Ltd., Korea United Pharm. Inc., Colorcon Co. Ltd., OPC Pharmaceutical JSC, Resantis Vietnam, and many other contributors and exhibitors for their generous support to make the conference successful.

We would like to thank all participants for your attendance and contribution to ASIAPHARM V and hope you all enjoy your time at this conference.

Respectfully yours,

THE ORGANIZING COMMITTEE

ASIAPHARM V
August 16th – 18th, 2023
Ton Duc Thang University, Ho Chi Minh City
VIETNAM

MESSAGE FROM THE HOST UNIVERSITY

Distinguished guests,
Ladies and Gentlements,

I am pleased to welcome all the distinguished speakers and participants of the 5th Asia Conference of Pharmaceutical Sciences (ASIAPHARM V), which is held at Ton Duc Thang University (TDTU), Vietnam, from August 16th to 18th, 2023. As the president of TDTU, I am delighted to host the ASIAPHARM V. It is an international scientific conference that offers a great opportunity to connect experts and researchers from various disciplines related to pharmaceutical sciences.

Ton Duc Thang University is a young and dynamic provider in the higher education sector and is one of the largest universities in Vietnam. The university is committed to Vietnam's sustainable development of human resources. It strives to be a leading research-oriented university regionally and internationally. We aim to create an environment that fosters quality education and empowers students in their learning and research pursuits.

On behalf of TDTU, I would like to extend my deepest gratitude to the plenary speakers, session chairs, organizing committee members, and participants who have contributed their time and expertise to make this conference possible. Additionally, I am deeply grateful to our great partners College of Pharmacy, Seoul National University (Korea), Bandung Institute of Technology (Indonesia), and Universiti Teknologi MARA (Malaysia). Furthermore, I would like to thank the track chairs and reviewers for their detailed comments and valuable suggestions. I believe this Conference will enrich our knowledge and forge lasting connections and collaboration among the attendees. Lastly, I hope that you will have a wonderful time exploring the beautiful city-Ho Chi Minh City.

I wish you all a successful and enjoyable conference. Thank you very much.

August 2023
Tran Trong Dao, Ph.D.
President
Ton Duc Thang University, Vietnam

ORGANIZERS AND COMMITTEES

Honorary Chairman:

Dr. Tran Trong Dao, President of Ton Duc Thang University, Vietnam

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- Prof. Abu Bakar Abdul Majeed, Faculty of Pharmacy, Universiti Teknologi MARA, Malaysia
- Prof. I Ketut Adnyana, School of Pharmacy, Bandung Institute of Technology, Indonesia

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Co-organizers:

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- Faculty of Pharmacy, Universiti Teknologi MARA, Malaysia
- School of Pharmacy, Bandung Institute of Technology, Indonesia

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- Prof. I Ketut Adnyana, School of Pharmacy, Bandung Institute of Technology, Indonesia

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- Prof. Nguyen Minh Duc, Faculty of Pharmacy, Ton Duc Thang University, Vietnam
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- Prof. Hiroyuki Morita; Institute of Natural Medicine, Toyama University, Japan
- Prof. Shin Jae-Gook; College of Medicine, Inje University, Korea
- Prof. Abu Bakar Abdul Majeed, Faculty of Pharmacy, Universiti Teknologi MARA, Malaysia
- Prof. Fazlin Mohd Fauzi, Faculty of Pharmacy, Universiti Teknologi MARA, Malaysia
- Prof. Daryono Hadi Tjahjono, School of Pharmacy, Bandung Institute of Technology, Indonesia
- Prof. Tran Thanh Dao, Faculty of Pharmacy, University of Medicine and Pharmacy Ho Chi Minh City, Vietnam
- Prof. Le Minh Tri, School of Medicine, Vietnam National University Ho Chi Minh City, Vietnam
- Prof. Nguyen Hai Nam, Hanoi University of Pharmacy, Vietnam
- Prof. Nguyen Thi Hoai, Faculty of Pharmacy, Hue University of Medicine and Pharmacy, Vietnam
- Assoc. Prof. Sornkanok Vimolmangkang, Faculty of Pharmaceutical Sciences, Chulalongkorn University, Thailand

- Assoc. Prof. Nguyen Minh Khoi, National Institute of Medicinal Materials Hanoi, Vietnam
- Assoc. Prof. Tran Viet Hung, National Institute of Drug Quality Control Ho Chi Minh City, Vietnam
- Assoc. Prof. Doan Cao Son, National Institute of Drug Quality Control Hanoi, Vietnam
- Assoc. Prof. Pham Thanh Suol, Faculty of Pharmacy, Can Tho University of Medicine and Pharmacy, Vietnam
- Dr. Nguyen Truong Huy, Faculty of Pharmacy, Ton Duc Thang University, Vietnam
- Dr. Nguyen Dang Thoai, Faculty of Pharmacy, Pham Ngoc Thanh Medical University Ho Chi Minh City, Vietnam
- Dr. Nguyen Minh Hien, Faculty of Pharmacy, Ton Duc Thang University, Vietnam
- Dr. Thach Ut Dong, Faculty of Pharmacy, Ton Duc Thang University, Vietnam
- Dr. Le Quoc Viet, Faculty of Pharmacy, Ton Duc Thang University, Vietnam
- Dr. Le Thuy Huong, Faculty of Pharmacy, Ton Duc Thang University, Vietnam
- Mr. Vu Huynh Kim Long (MSc.), Faculty of Pharmacy, Ton Duc Thang University, Vietnam

Conference Secretary:

Dr. Le Quoc Viet, Faculty of Pharmacy, Ton Duc Thang University, Vietnam

CONFERENCE INFORMATION

DATE AND VENUE

August 16th – 18th, 2023
Ton Duc Thang University
19 Nguyen Huu Tho Street, Tan Phong Ward, District 7, Ho Chi Minh City, Vietnam
Phone: (+84) 8 37761043
Hotline: (+84) 9 09 04 11 90
Email: asiapharmV@tdtu.edu.vn

RECEPTION DESK

The reception desk is located on the Ground floor of Building A and opens from 7:00 to 17:30 from August 17th to 18th, 2023.

LANGUAGE

All sessions will be presented in English.

NAME TAG/BADGES

Admittance to the venue is restricted to participants wearing their name badges. Wearing badges is compulsory both inside the venue and at all events organized with its context.

CONFERENCE ROOM'S LOCATION

The Conference will be held in the conference rooms at Buildings A, B, C, and F.

CONFERENCE ROOM'S EQUIPMENT

Each conference room will be equipped with an overhead projector and a notebook computer.

RULES OF PROCEDURE FOR MEETING

It takes 15 minutes for each oral presentation. Each paper will be presented orally for 10 minutes, followed by about 5 minutes for discussion. Speakers will be noticed by the Chairman of session 5 minutes before ending.

POSTER PRESENTATION TIME

Presentation time: August 17th, 2023: 16:20-17:30
Award: August 18th, 2023: 12:00
Venue: Lobby 2A (Building A)
Each poster will have a billboard dimension of 90 cm × 120 cm (width × length) and should be presented by the presenting person at designated periods in the assigned area.

EXHIBITION

Hall C, and Exhibition series G (at the internal road N0.01).

LUNCH

Buiding D, 11th and 12th floors

GALA DINNER

The Adora Premium, 803 Nguyen Văn Linh St., Tan Phu Ward, District 7, Ho Chi Minh City

TRANSPORTATION

Tan Son Nhat International Airport ➔ Ton Duc Thang University (TDTU)
By taxi: It takes about USD 15-20, and about 45 minutes to arrive at Ton Duc Thang University.

- Taxi Mai Linh: https://mailinh.vn/
- Taxi Vinasun: https://vinasun.vn/
- Grab, Gojek transportation services are also available in Ho Chi Minh City

PARKING

Participants with the conference invitation can park their cars at campus parking lots.

ACCOMODATION (FOR FULL-FEE REGISTRATION): CONTACT

ibis Saigon South , 73 Hoang Van Thai Street, Tan Phu Ward, District 7, Ho Chi Minh City, Vietnam

CONFERENCE MAP

For general inquiries:

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For sponsorship and exhibition:

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Faculty of Pharmacy, Ton Duc Thang University, Ho Chi Minh City, Vietnam.
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AGENDA AT A GLANCE

AUGUST 17TH, 2023

Timeline	Topic	Location
7:00 - 8:30	**Registration**	**Lobby A**
8:30 - 9:00	**Opening Ceremony**	**Hall 2A**
9:00 - 9:30	**Tea break & Poster Visiting**	**Lobby A**
	Plenary Lecture *Chairs: Prof. Minh Duc Nguyen - Prof. Sang Kook Lee*	**Hall 2A**
9:30 - 10:00	*Vietnam Pharma Industry Status and Development Strategy for Pharmaceutical Sector to 2030, Vision to 2045* Van Truyen Le, Ministry of Health of Vietnam	
10:00 - 10:30	*Structural Study on Toxin-Antitoxin Systems in Pathogenic Bacteria: a Target for Developing Antimicrobial Agents* Bong Jin Lee, Seoul National University, Korea	
10:30 - 11:00	*Clinical Implementation of Personalized Precision Pharmacotherapy based on Pharmacogenomics* Jae Gook Shin, Inje University, Korea	
11:00 - 11:30	*Engineering of Biosynthetic Enzymes to Synthesize Bioactive Compounds* Morita Hiroyuki, University of Toyama, Japan	
11:30 – 13:30	**Lunch & Poster Visiting**	
13:30 - 16:20	**Scientific Sessions**	
	Session 1: Organic and Medicinal Chemistry	**A101**
	Session 2: Pharmacology and Clinical Pharmacy	**A104**
	Session 3: Pharmaceutics and Industry Pharmacy	**B010**
	Session 4: Pharmacognosy and Natural Products	**C010**
	Session 9: Young Scientists	**B106**
16:20 – 17:30	**Posters Visiting**	
19:00 – 21:00	**Gala dinner**	

AUGUST 18TH, 2023

Timeline	Topic	Location
	Scientific Sessions	
8:00 - 9:30	**Session 5:** Pharmaceutical Biotechnology	
	Session 6: Pharmaceutical Management and Economics	**A101**
	Session 7: Pharmaceutical Analysis and Quality Control	**A104**
	Session 8: Multimodality Drug Development	**B010**
		C010
9:30 – 10:00	**Tea break & Poster Visiting**	**Lobby A**
	Plenary Lecture *Chairs: Prof. Morita Hiroyuki - Prof. Shir-ly Huang*	**Hall 10F**
10:00 - 10:30	*Redox Regulation of Cellular Stress Response* Young-Joon Surh, Seoul National University, Korea	
10:30 - 11:00	*Fifty years of Vietnamese Ginseng's Discovery: Research advance, challenge and prospect.* Minh Duc Nguyen, Ton Duc Thang University, Vietnam	

11:00 - 11:30	*Microbiota-Based Therapy and Health Promotion Focusing on Lactate Metabolism* Shir-ly Huang, National Yang Ming Chiao Tung University, Taiwan	
11:30 - 12:00	*Rational Design and Development of Potent Glutaminyl Cyclase (QC) Inhibitors as Anti-Alzheimer's Disease* Jee Woo Lee, Seoul National University, Korea	
12:00	**Closing ceremony** **Poster Award** **Closing Speech**	

AGENDA OF SCIENTIFIC PROGRAM

August 17th, 2023

SS1: Organic and Medicinal Chemistry **Room A101**

Chairs: Daryono Hadi Tjahjono, Bandung Institute of Technology, Indonesia
Supakarn Chamni, Chulalongkorn University, Thailand

Secretary: Ut Dong Thach, *Ton Duc Thang University, Vietnam*

Timeline	Topic
13:30 - 13:45	<OMC-01> Metal-free synthesis of potential physiologically active 4-imidazolidinones from cheap chemical feedstocks **Dung T. Do**, The Citadel Military College of South Carolina, USA
13:45 - 14:00	<OMC-02> Screening and Evaluation of Novel Bioactive Peptides for Dipeptidyl Peptidase - IV and Angiotensin-Converting Inhibitory Activity **Nong Thi Phuong Nhung**, Thainguyen University of Agriculture and Forestry, Vietnam
14:00 - 14:15	<OMC-03> Anti-osteoporosis properties of xanthones from Garcinia plants **Ut Dong Thach**, Ton Duc Thang University, Vietnam
14:15 - 14:30	<OMC-04> Hydrocinamic acid derivatives as the promising steroid 5a-reductase inhibitors **Supakarn Chamni**, Chulalongkorn University,Thailand
15:00 - 15:15	<OMC-05> Design, synthesis and biological evaluation of novel alkoxy/hydroxyaurones as potent pancreatic inhibitors **Cam-Van Vo**, University of Medicine and Pharmacy at Ho Chi Minh city, Vietnam
15:15 - 15:30	<OMC-06> Bridging Nature and Technology: The Synergy of Natural Products and Artificial Intelligence Fazlin Mohd Fauzi, Universiti Teknologi MARA, Malaysia
15:30 - 15:45	<OMC-07> The α-glucosidase Inhibitory Activity of Avicularin and 4-O-methyl gallic Acid Isolated from Syzygium myrtifolium leaves **Muhamad Insanu**, Bandung Institute of Technology, Indonesia
15:45 - 16:00	<OMC-08> In Silico discovery of dual AChE and BACE1 inhibitors for Alzheimer's disease **Do Thi Mai Dung**, Hanoi University of Pharmacy, Vietnam

SS2: Pharmacology and Clinical Pharmacy **Room A104**

Chairs: Baohong Jiang, *Shanghai Institute of Materia Medica, China*
Varalee Yodsurang, *Chulalongkorn University, Thailand*

Secretary: Thuy Huong Le, *Ton Duc Thang University, Vietnam*

Timeline	Topic
13:30 -13:45	<PCP-01> Drug development based on traditional Chinese medicine **Baohong Jiang**, Shanghai Institute of Materia Medica, China
13:45-14:00	<PCP-02> Emerging concepts in rheumatoid arthritis: the story from proton-sensing receptors **Wei-Hsin Sun**, National Yang Ming Chiao Tung University, Taiwan
14:00 -14:15	<PCP-03> Identification of diagnostic biomarkers for ovarian cancer: bench to bedside **Varalee Yodsurang**, Chulalongkorn University, Thailand

Timeline	Topic
14:15-14:30	<PCP-04> Study on the antibacterial, antioxidant and hypergycemia-preventive effects of Lactuca indica L.-Asteraceae **Tran Thi Thu Hong**, Hong Bang International University, Vietnam
15:00 -15:15	<PCP-05> Extract from Hymenopellis radicata inhibits the growth of 4T1 cancer cells **Nguyen Thi Kim Anh**, Industrial University of Ho Chi Minh City, Vietnam
15:15 -15:30	<PCP-06> Sulforaphane regulates eNOS activation and NO production via Src-mediated PI3K/Akt signaling in human endothelial EA hy926 cells **Pham Ngoc Khoi**, Pham Ngoc Thach University of Medicine
15:30 -15:45	<PCP-07> In vivo antidiarrheal effect of Andaliman (Zanthoxylum acanthopodium dc.) fruit ethanol extract **Maria Immaculata Iwo**, Institut Teknologi Bandung, Indonesia
15:45 -16:00	<PCP-08> Insulin-like growth factor binding protein-3 exerts its anti-metastatic effect in aerodigestive tract cancers by disrupting the protein stability of vimentin **Thuy Huong Le**, Ton Duc Thang University, Vietnam

SS3: Pharmaceutics & Industrial Pharmacy
Room B010
Chairs: Chuda Chittasupho, *Chiang Mai University, Thailand*
Quoc-Viet Le, *Ton Duc Thang University, Vietnam*
Secretary: **Quoc-Viet Le,** *Ton Duc Thang University, Vietnam*

Timeline	Topic
13:30 - 13:45	<PIP-01> External stimuli-responsive drug delivery systems for in situ vaccination **Gayong Shim**, Soongsil University, Korea
13:45 - 14:00	<PIP-02> Lysyl oxidase-responsive anchoring nanoparticles for modulation of the tumor immune microenvironment **Jaiwoo Lee**, Seoul National University, Korea
14:00 - 14:15	<PIP-03> Dextran nanoparticle: a versatile nanocarrier for the delivery of therapeutic oligonucleotides **Nguyen Van Hien**, Van Lang University, Vietnam
14:15 - 14:30	<PIP-04> Mesoporous silica particles as versatile platform for immunotherapy **Thanh Loc Nguyen**, Sungkyunkwan University, Korea
15:00 -15:15	<PIP-05> Jelly loaded with nanogel containing Mucuna pruriens seed extract for neuroprotection in Parkinson's disease **Chuda Chittasupho**, Chiang Mai University, Thailand
15:15 -15:30	<PIP-06> Polydopamine - A versatile biomaterial for drug delivery systems in cancer immunotherapy **Quoc-Viet Le**, Ton Duc Thang University, Vietnam
15:30 -15:45	<PIP-07> Development of Couette-Taylor crystallizer applied in the pharmaceutical industry **Anh-Tuan Nguyen**, Ton Duc Thang University, Vietnam

SS4: Pharmacognosy & Natural Products **Room C010**

Chairs: Seikwan Oh, *Ewha Womans University, Korea*
Sornkanok Vimolmangkang, *Chulalongkorn University, Thailand*
Secretary: Hien Minh Nguyen, Ton Duc Thang University, Vietnam

Timeline	Topic
13:30 -13:45	<PNP-01> Production of cannabis hairy root and its elicitation for enhancement of triterpenoids **Sornkanok Vimolmangkang**, Chulalongkorn University, Thailand
13:45-14:00	<PNP-02> Cytotoxicity activity, metabolite profiling, and isolation compound from crude hexane extract of Cleome rutidospermae **Budiman Yasir**, Sekolah Tinggi Ilmu Farmasi Makassar, Indonesia
14:00 -14:15	<PNP-03> Eriodictyol attenuates H O -induced oxidative damage in human dermal fibroblasts through enhanced capacity of antioxidant machinery **Visarut Buranasudja**, Chulalongkorn University, Thailand
14:15-14:30	<PNP-04> Integrative approaches for the identification of suspicious forensic plant specimens from life threatening case in Thailand **Aekkhaluck Intharuksa**, Chiang Mai University, Thailand
15:00 - 15:15	<PNP-05> Evaluation of the antioxidant and anti-tyrosinase effects of Ochna integerrima flowers **Hien Minh Nguyen**, Ton Duc Thang University, Vietnam
15:15 - 15:30	<PNP-06> Enantiomer and Anti-Glioma Properties of MMEO Compound (3'-metoxy- 3'',4''(Metilendioxy)- 2,5-Epoxilignan-4ol-6one **Yusnita Rifai**, Hasanuddin University, Indonesia
15:30 - 15:45	<PNP-07> Crystal structural analysis of norbelladine 4'-O-methyltransferase **Saw Yu Yu Hnin**, University of Toyama, Japan
15:45 - 16:00	<PNP-08> Melatonin inhibits chondrosarcoma cell proliferation and metastasis by enhancing miR-520f-3p production and suppressing MMP7 expression **Nguyen Bao Tran**, China Medical University, Taiwan
16:00 - 16:45	<PNP-09> Chinese herbal medicine alleviating muscle atrophy in murine myoblasts via the anti-inflammatory effects **Lin-Chu Huang**, China Medical University, Taichung, Taiwan

SS9: Young Scientists **Room B106**

Chairs: **Thien Y Vu,** Ton Duc Thang University, Vietnam
Duc Toan Pham, Ton Duc Thang University, Vietnam

Timeline	Topic
13:30 - 13:45	<YC-01> Ligand-based pharmacophore modeling and molecular docking studies of Akt2 inhibitors from marine natural product database **Zenith Putri Dewianti**, Bandung Institute of Technology, Indonesia
13:45 - 14:00	<YC-02> Reviewing the roles of glutathione peroxidase-1 gene on addictive effects induced by cocaine in gene-manipulating mouse model. **Duc Toan Pham**, Ton Duc Thang University, Vietnam
14:00 - 14:15	<YC-03> Insight into the structure and physicochemical properties of potent chemokine receptor 5 inhibitors in the discovery of novel Alzheimer's disease drugs **Nur Intan Saidaah Mohamed Yusof**, Universiti Teknologi MARA, Malaysia

Timeline	Topic
14:15 - 14:30	<YC-04> A survey on neuropathic pain medications dosages prescribed by traditional medicine practitioners in diabetic peripheral neuropathy treatment **Nguyen Thi Kim Nhan**, University of Medicine and Pharmacy in Ho Chi Minh City, Vietnam
15:00 - 15:15	<YC-05> Quality of life and associated factors among patients with diabetes mellitus at the Thong Nhat hospital, Viet Nam **Trang Vu Thi**, Vietnam National University, Vietnam
15:15 - 15:30	<YC-06> Association between SLC22A1 gene polymorphisms and the efficacy of tyrosine kinase inhibitors as treatment for chronic myeloid leukemia: A systematic review and meta-analysis **Vu Thi Thuy**, Ho Chi Minh University of Technology (HUTECH), Vietnam
15:30 - 15:45	<YC-07> Phagocytic Activity of Trigona Honey In Male Mice (Mus musculus) Using Carbon Clearance Method **Akbar Awaluddin**, Sekolah Tinggi Ilmu Farmasi (STIFA) Makassar, Indonesia
15:45 - 16:00	<YC-08> Phenotypic and molecular assessment on the pharmacological effects of Secang Wood (Caesalpinia sappan L.) extract in Drosophila melanogaster **Nur Rahma Rumata**, Sekolah Tinggi Ilmu Farmasi Makassar, Indonesia
16:00 - 16:15	<YC-09> Cytotoxic activity of red fruit (Pandanus conoideus Lam.) extract on cervical cancer cell line (Hela) **Dewi Purwaningsih**, Sekolah Tinggi Ilmu Farmasi Makassar, Indonesia
16:15 - 16:30	<YC-10> Caffeic acid derivatives inhibit osteoclast functioning, osteoporosis and osteolytic bone metastases **Le Huynh Hoai Thuong**, China Medical University, Taiwan

August 18th, 2023

SS5: Pharmaceutical Biotechnology **Room A101**

Chairs: **Nhat Tu Le,** Weill Cornell Medical College, U.S.A
Yei-Tsung Chen, National Yang Ming Chiao Tung University, Taiwan
Secretary: Bao Le, *Ton Duc Thang University, Vietnam*

Timeline	Topic
8:00 - 8:15	<PBT-01> Post-translational modifications, cellular senescence, and atherosclerotic cardiovascular disease **Nhat Tu Le**, Houston Methodist Research Institute, USA
8:15 - 8:30	<PBT-02> MicroRNA profiling in Vietnamese nasopharyngeal carcinoma and its application in nasopharyngeal cancer treatment **Thuan Duc Lao**, Ho Chi Minh City Open University, Vietnam
8:30 - 8:45	<PBT-03> Therapeutic potential of targeting Heart Failure (HF)-related microRNAs for HF treatment **Yei-Tsung Chen**, National Yang Ming Chiao Tung University, Taiwan
8:45 - 9:00	<PBT-04>Cannabinoid Compounds as Tyrosine Kinase Inhibitors Against Erb2 for Anticancer Therapy **Natharin Phattayanon**, Payap University, Thailand
9:00 -9:15	<PBT-05> Ganoderma microsporum immunomodulatory protein acts as a multifunctional broad-spectrum antiviral against SARS-CoV-2 by interfering virus binding to the host cells and spike-mediated cell fusion **Ngoc Kha Di Vo**, National Yang Ming Chiao Tung University, Taiwan

SS6: Pharmaceutical Management & Economics **Room A104**

Chairs: **Van Truyen Le,** Former Deputy Minister, Ministry of Health, Vietnam
Usa Chaikledkaew, Mahidol University, Thailand
Secretary: Xuan Nam Vo, *Ton Duc Thang University, Vietnam*

Timeline	Topic
8:00 - 8:15	<PME-01> Future challenges of health technology assessment on policy decision making in ASEAN countries: Lesson learnt from Thailand **Usa Chaikledkaew**, Mahidol University, Thailand
8:15 - 8:30	<PME-02> Reducing medication errors: The role of hospital pharmacists in hospital settings **Thuy Thi Thu Ngo**, Vinmec Central Park International Hospital, Vietnam
8:30 - 8:45	<PME-03> Health-related quality of life in patients with COVID-19 in Indonesia: A cross-sectional study **Fajriansyah**, Sekolah Tinggi Ilmu Farmasi, Indonesia
8:45 - 9:00	<PME-04> Economic Evaluation of Glucosamine in Knee Osteoarthritis Treatments in Vietnam: A Preliminary Results **Nam Xuan Vo**, Ton Duc Thang University, Vietnam

SS7: Pharmaceutical Analysis & Quality Control **Room B010**

Chairs: **Duc Tuan Nguyen**, University of Medicine and Pharmacy, Vietnam
JiSuk Lee, Seoul National University, Korea

Secretary: Truong Huy Nguyen, *Ton Duc Thang University, Vietnam*

Timeline	Topic
8:00 - 8:15	<PAQ-01> Triterpene esters from Uncaria rhynchophylla hooks are able as new selective inhibitors on HIV-1 protease and their molecular docking study **JiSuk Lee**, Seoul National University, Korea
8:15 - 8:30	<PAQ-02> Structure characterization and immunoregulatory effect of cell wall polysaccharides from Pu-erh tea on RAW264.7 cells by JAK/STAT pathway **Jing Li**, Shanghai Normal University, China
8:30 - 8:45	<PAQ-03> UPLC-QTOF-MS based metabolomics approach for the authentication of Panax vietnamensis var fuscidiscus and Panax vietnamensis var vietnamensis **Huy Truong Nguyen**, Ton Duc Thang University, Vietnam
8:45 - 9:00	<PAQ-04> Advancing personalized medicine for tuberculosis with multi-modal metabolomics and lipidomics **Nguyen Phuoc Long**, Inje National University, Korea
9:00 - 9:15	<PAQ-05> Potency of Bioactive Compounds from Caulerpa racemosa in Handling Diabetes-Related Complications: ADMET Properties and Molecular Docking Simulations **Muhammad Aswad**, Hasanuddin University, Indonesia

SS8: Multimodality drug development **Room C010**

Chairs: Byung Hoon Lee, *Seoul National University, Korea*

Secretary: Bich Hang Do, *Ton Duc Thang University, Vietnam*

Timeline	Topic
8:00 - 8:15	<MDD-01> Development of RORα agonists for the treatment of metabolic disorders **Hyeung-geun Park**, Seoul National University, Korea
8:15 - 8:30	<MDD-02> Structure-Activity Relationship (SAR) study of novel nucleoside A2A adenosine receptor antagonist as immune-oncology agents **Lak Shin Jeong**, Seoul National University, Korea
8:30 - 8:45	<MDD-03> Development of therapeutic cancer vaccine against acute myeloid leukemia **Yeonseok Chung**, Seoul National University, Korea
8:45 - 9:00	<MDD-04> Computer-aided drug discovery: From small compounds to protein inhibitors against tyrosine kinase of EGFR for cancer therapy **Kiattawee Choowongkomon**, Kasetsart University, Thailand

PLENARY LECTURES

August 17th, 2023

Chairs: Prof. Dr. Minh Duc Nguyen, Ton Duc Thang University, Vietnam
Prof. Dr. Sang Kook Lee, Seoul National University, Korea

PL-01 Vietnam pharma industry status and development strategy for pharmaceutical sector to 2030, vision to 2045
Le Van Truyen, Ministry of Health of Vietnam

PL-02 Structural study on toxin-antitoxin systems in pathogenic bacteria: a target for developing antimicrobial agents
Bong-Jin Lee, Seoul National University, Korea

PL-03 Clinical implementation of personalized precision pharmacotherapy based on pharmacogenomics
Jae-Gook Shin, Inje University, Korea

PL-04 Engineering of biosynthetic enzymes to synthesize bioactive compounds
Hiroyuki Morita, University of Toyama, Japan

August 18th, 2023

Chairs: Prof. Dr. Hiroyuki Morita, University of Toyama, Japan
Prof. Shir-Ly Huang, National Yang Ming Chiao Tung University, Taiwan

PL-05 Redox regulation of cellular stress response
Young-Joon Surh, Seoul National University, Korea

PL-06 Fifty years of Vietnamese ginseng's discovery: Research advance, challenge and prospect
Minh Duc Nguyen, Ton Duc Thang University, Vietnam

PL-07 Microbiota-based therapy and health promotion focusing on lactate metabolism
Shir-Ly Huang, National Yang Ming Chiao Tung University, Taiwan

PL-08 Rational design and development of potent glutaminyl cyclase inhibitors as anti-Alzheimer's agents
JeeWoo Lee, Seoul National University, Korea

<PL-01>

Vietnam pharmaceutical sector status and the development strategies to the year 2030 with vision to 2045

Le Van Truyen

Senior Expert
Former Vice Minister of Health
Vietnam Ministry of Health

The author presents and highlights the important documents of Vietnam Government on strategies for development of pharmaceutical sector in 30' decade, with vision to 2045.
The presentation also gives an overview on recent status and achievements of Vietnam Pharma Industry in the last decade. The expectable position of Vietnam pharmaceutical industry for 30' decade was analyzed based on the policies and strategies established in relevant resolutions of the Government of Vietnam. The challenges in the development process of Vietnam Pharma Industry have been critically analyzed. The factors impacting into the process of modernization of Vietnam pharmaceutical industry were discussed and suggested for realization of the objectives of the Vietnam pharmaceutical industry development in the context of fierce competition in the process of economic globalization to the ASEAN region and the world.

<PL-02>

Structural study on toxin-antitoxin systems in pathogenic bacteria: A target for developing antimicrobial agents

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Keywords: bacteria, recombinant protein, vaccine

Abstract

The bacterial toxin – antitoxin (TA) system is a module that may play a role in cell survival under stress conditions. Generally, toxin molecules act as negative regulators in cell survival and antitoxin molecules as positive regulators. Thus, the expression levels and interactions between toxins and antitoxins should be systemically harmonized so that bacteria can escape such harmful conditions. Since TA systems are able to control the fate of bacteria, they are considered as potent targets for the development of new antimicrobial agents. TA systems are widely prevalent systems existing in bacteria: there are eight types of bacterial TA systems depending on the property of the antitoxin which binds either the protein toxin or mRNA coding the toxin protein. Moreover, the multiplicity of TA genes has been observed even in species of bacteria. Therefore, knowledge on TA systems such as the individual characteristics of TA systems, integrative working mechanisms of various TA systems in bacteria, interactions between toxin molecules and cellular targets, and so on is currently limited due to their complexity. In this regard, it would be helpful to know the structural characteristics of TA modules for understanding TA systems in bacteria. Here, we present the structural information of TA systems by using NMR, X-ray crystallography and Cryo-EM and suggest antibiotics candidates which inhibit the interaction between Toxin and Antitoxin proteins from infectious bacteria, especially focusing on the TA modules of *Mycobacterium Tuberculosis, Streptococcus pneumoniae etc.*

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<PL-03>

Clinical implementation of personalized precision pharmacotherapy based on pharmacogenomics

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Keywords: precision medicine, pharmacogenomics, clinical implementation, CDSS

It is well known dogma of pharmacology that therapeutic drug response varies among the individual patients from the same therapeutic dose regimen. The drug response variation caused by many factors of individual subjects such as personal genes, drug interaction, age, body weight renal/hepatic dysfunction, ethnicity etc. The personalized precision medicine based on an individual pharmacogenotypes has been already established in the clinical practice, at least in some therapeutic areas including the treatment of cancer, cardiovascular diseases, psychiatric drugs and prevention of serious adverse drug reactions. Therefore, these approaches are well agreed by the global consortium of pharmacogenomics implementation in clinical practice, and those serviced are covered by insurance coverage for reimbursement.

The genotype guided personalized dose regimen is available to be predicted from the clinical documents collected from clinical trials/ studies done in an individual with specific pharmacogenotypes. However, this approach may not be available for such edge population patients who are exposed to many other clinical conditions such as combined effect of genetic and non-genetic effects, i.e. genetic + drug interactions + renal dysfunction + old age. Therefore, it is asked to have additional solutions to predict the personalized precision dosing of an individual patients exposed to diverse clinical situation in real world clinical practice and model informed precision dosing (MIPD) will be a potential solution in the near future.

The presentation will introduce the real world practice of personalized pharmacotherapy based on pharmacogenotypes of an individual patient and also MIPD as a potential tool for coming precision dosing of real world edge patient population.

<PL-04>

Engineering of biosynthetic enzymes to synthesize bioactive compounds

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Keywords: Cannabinoid, Olivetolic acid cyclase, X-ray crystal structure

About 60% of the present drugs were developed from natural products with unique chemical diversity and biological activities. Hence, discovery of new bioactive compounds from natural products is still important for the drug development. On the other hand, breakthrough made in synthetic biology has also begun to supply us with many useful compounds through manipulation of biosynthetic genes for secondary metabolites. Theoretically, this approach can be also exploited to generate new unnatural compounds by intermixing genes from different biosynthetic pathways.
Considering the potential, we are studying about engineering of the secondary metabolite enzymes to expand their substrate and product specificities. In this presentation, structure-based dual engineering of olivetolic acid cyclase (OAC) and tetraketide synthase (TKS) responsible for the formation of the resorcinol core of tetrahydrocannabinoid, will be mainly discussed. In brief, the study successfully expanded the substrate specificities of both enzymes, to produce olivetolic acid analogs with longer alkyl-chain at C-3. The findings provide beneficial insights into the further development of various alkyl cannabinoid analogs by synthetic biological approaches.

<PL-05>

Redox regulation of cellular stress response

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Keywords: Cellular stress response, NRF2, Redox regulation

Living organisms have evolved ubiquitous mechanisms to manage a vast multitude of stressors and noxious conditions. One central player in cellular adaptive stress response is the nuclear factor erythroid 2 p45-related factor (NRF2). This transcription factor regulates the expression of a battery of antioxidant enzymes and other cytoprotective proteins, thereby maintaining cellular redox homeostasis. Some chemoprotective and chemopreventive phytochemicals are capable of activating NRF2 signaling. However, redox homeostasis is not only essential for the maintenance of normal physiological functions, but also plays an important role in the growth, survival, and therapy resistance of cancer cells. Redox imbalance and consequent disruption of redox signaling are implicated in the proliferation and progression of cancer cells and their resistance to chemo- and radio-therapy. Aberrant NRF2 overactivation has been observed in many cancerous and transformed cells. Uncontrolled amplification of NRF2-mediated antioxidant signaling results in reductive stress. Some metabolic pathways altered due to reductive stress have been identified as major contributors to tumorigenesis. This lecture will highlight the multifaceted roles of NRF2 as both tumor suppressive and prooncogenic proteins.

<PL-06>

Fifty years of Vietnamese ginseng's discovery - research advance, challenge and prospect

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Keywords: Vietnamese ginseng, *Panax vietnamensis*, Research advance-challenge-prospect

Vietnamese ginseng (VG), *Panax vietnamensis* Ha *et* Grushv. (PVV), was a new and the southernmost *Panax* species discovered in Middle Vietnam in 1973. Since then, VG has been systematically studied on many aspects including botany, taxonomy, chemistry, biology, pharmacology, etc. VG posseses a characteristic saponin composition with more than 60 kinds of saponins. In addition, the saponin content of VG is very high (up to 15-20%) compared with other *Panax* spp. Besides oleanolic acid, protopanaxadiol and protopanaxatriol ginsenosides as in Korean ginseng (*Panax ginseng* C.A. Meyer), VG contains lots of ocotillol-type saponins, of which majonoside-R2 is the major one (yield over 5%). VG showed similar biological and pharmacological activities with those of Korean ginseng such as tonic and adaptogenic effects, enhancing physical performance and vitality, reducing fatigue, etc. In addition, VG and its major saponin M-R2 showed remarkable anti-stress effects. M-R2 was also proven to have *in vitro* and *in vivo* anti-tumor activity. VG was officially added to the list of Vietnam national products in 2017.

Despite its high value and large market demand, in fact the development of VG is currently facing significant difficulties and challenges. Traditional cutivation practices under natural forest canopy lead to low productivity, insufficient supply to the market, and expensive price of VG that are unaffordable for most comsumers. Accidental confusion or deliberate adulteration of VG with some other *Panax* species, especially with Ye sanchi (*Panax vietnamensis* var. *fuscidiscus* – PVF) has created a unstable VG market while effective management and quality control measures remain inadequate. The quantity and quality of reasearch works on VG are still limited compared to those of famous *Panax* spp., such as Korean ginseng and Sanchi ginseng.

However, recent governmental policies including the program for national products development, the recent decision on the development program for VG until 2030 with a vision to 2045, etc., have created an important new motivation for the development of VG. In addition, strong and increasing investment of businesses and farmers in the field of cultivation, R&D, and finished-product manufacturing has shaped a promising future for VG.

On the occasion of the fiftieth year of VG's dicovery, this presentation will provide an updated review on scientific advances, highlight challenges in market and scientific development, as well as outline the prospect of VG, a national treasure of Vietnam.

<PL-07>

Microbiota-based therapy and health promotion focusing on lactate metabolism

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Over the past two decades, the human microbiota were found to have important roles in health maintenance. *Veillonella* spp. are obligately anaerobic, Gram-negative bacteria found in the human oral cavity and gut. They belong to Bacillota and Veillonellaceae. Recent studies have indicated that gut *Veillonella* promote human homeostasis by utilizing lactate as main carbon source and producing beneficial metabolites. The health promoting metabolites include propionate, acetate, tryptophan-derivatives and NO_2^-/NO. The gut lumen is a dynamic environment with fluctuating nutrient levels, so the microbes exhibit shifting growth rates with significant gene expression. Current knowledge of *Veillonella* lactate metabolism has focused on log phase growth. However, most of the time the gut microbes are in the stationary phase. The global gene expression was demonstrated that *V. dispar* reprograms during growth phases on lactate to explain the metabolites production during stationary phase. The relationship between mucin-binding probiotics and *Veillonella* species were systemically paired and demonstrated some pairs are mutual. The physical interaction of the two types of bacteria was observed. *V. dispar* produced about threefold higher levels of acetate and propionate, in the co-culture with lactobacilli. Our interbacterial studies, combining traditional and next generation probiotics, provide a better understanding of human health-promoting mechanism. As the lactic acidosis causing neural toxicity, inflammation and promoting cancer metastasis, our cross-feeding lactate-utilizing bacterial strategy can be applied as potential microbiota-based therapies.

<PL-08>

Rational design and development of potent glutaminyl cyclase inhibitors as anti-Alzheimer's agents

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The pyroglutamate form of Aβ (pE-Aβ), a posttranslational product of *N*-truncated Aβ peptides, comprises a substantial proportion of Aβ peptides, accounting for more than 50% of the total Aβ plaques in the AD brain. pE-Aβ is a major constituent of Aβ species deposited in early extracellular plaques and intraneuronal aggregates. Many studies report that pE-Aβ is found upstream of the amyloid cascade, contributing to the early stages of AD pathogenesis and ultimately leading to clinical dementia. Compared with unmodified Aβ, pE-Aβ species exhibit a higher propensity for aggregation and participate in plaque seeding rather than in the formation of oligomeric and fibrillar Aβ assemblies. Furthermore, pE-Aβ aggregates not only exhibit higher neuronal and glial toxicities but also demonstrate greater resistance to proteolytic degradation by peptidases. In addition, pE-Aβ contributes to the formation of hyperphosphorylated tau, suggesting a possible connection between the two neurotoxic species in AD. In a recent clinical trial, patients exhibiting early symptoms of AD were treated with donanemab, a monoclonal antibody to pE-Aβ and the treatment resulted in a significant slowing of decline in cognition and daily function, supporting that pE-Aβ is an alternative therapeutic target for AD.

Glutaminyl cyclase (QC), belonging to the family of metal-dependent aminoacyltransferases, is responsible for the conversion of glutaminyl (Q) or glutamyl (E) residues at the terminus of peptides into the corresponding g-lactam ring and is mainly found in the hippocampus and cortex of the mammalian brain. In Aβ peptides, QC catalyzes the conversion of the *N*-truncated Aβ peptide ($A\beta_{3\text{-}40/42}$) generated from $A\beta_{40\text{-}42}$ by dipeptidyl peptidase IV into the pyroglutamate peptide $pE_3\text{-}A\beta_{40/42}$. QC protein and mRNA levels are higher in the brains and cerebrospinal fluid of AD patients than in control brains and can be detected in the early stages of AD. Furthermore, QC knockout has been shown to rescue cognitive function in AD model mice, and QC inhibitors efficiently reduce the levels of pE_3-Aβ and Aβ plaques in the brain, improving memory deficits in AD mice. These findings support QC inhibition as a viable therapeutic strategy for AD.

Recently, we have investigated new classes of QC inhibitors designed by bioisostere-based, pharmacophore-based and structure-based approaches, respectively, of which the selected inhibitors exhibited extremely potent QC inhibition compared to PQ912, a Phase 2 QC inhibitor. In vivo studies demonstrated that they significantly reduced the concentrations of pE_3-Aβ and total Aβ in the brain and restored cognitive functions in AD animal models. In addition, further pharmacokinetic and toxicity studies indicated that they had drug-like properties as preclinical candidates. In this presentation, I will present our recent studies on the discovery of potent QC inhibitors rationally designed.

ORAL PRESENTATIONS

SESSION 1. Organic & Medicinal Chemistry

Chairs: **Daryono Hadi Tjahjono, Bandung Institute of Technology, Indonesia**
Supakarn Chamni, Chulalongkorn University, Thailand
Secretary: **Ut Dong Thach, Ton Duc Thang University, Vietnam**

OMC-01 Metal-free synthesis of potential physiologically active 4-imidazolidinones from cheap chemical feedstocks
Dung T. Do, The Citadel Military College of South Carolina, USA

OMC-02 Screening and evaluation of novel bioactive peptides for simultaneously down-regulating activities of dipeptidyl peptidase - iv and angiotensin-converting enzyme
Nong Thi Phuong Nhung, Thainguyen University of Agriculture and Forestry, Vietnam

OMC-03 Anti-osteoporosis properties of xanthones from *Garcinia* plants
Ut Dong Thach, Ton Duc Thang University, Vietnam

OMC-04 Hydrocinamic acid derivatives as the promising steroid 5α reductase inhibitors
Supakarn Chamni, Chulalongkorn University, Thailand

OMC-05 Design, synthesis and biological evaluation of novel alkoxy/hydroxyaurones as potent pancreatic inhibitors
Cam-Van Vo, University of Medicine and Pharmacy at Ho Chi Minh city, Vietnam

OMC-06 Bridging nature and technology: The synergy of natural products and artificial intelligence
Fazlin Mohd Fauzi, Universiti Teknologi MARA, Malaysia

OMC-07 The α-glucosidase Inhibitory Activity of Avicularin and 4-O-methyl gallic Acid Isolated from *Syzygium myrtifolium* leaves
Muhamad Insanu, Bandung Institute of Technology, Indonesia

OMC-08 *In Silico* discovery of dual AChE and BACE1 inhibitors for Alzheimer's disease
Do Thi Mai Dung, Hanoi University of Pharmacy, Vietnam

<OMC-01>

Metal-free synthesis of potential physiologically active 4-imidazolidinones from cheap chemical feedstocks

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Keywords: Hidden Sub-catalysis, Metal-free synthesis, one-pot cascade reactions, heterocyclic

Background: Nitrogen-based heterocycles hold a unique and significant role in medicinal chemistry as a rich source of therapeutic agents. They are highly valued, with over 75% of FDA-approved drugs and currently available medications containing nitrogen-containing heterocyclic structures. Furthermore, it is expected that an even larger proportion of newly developed pharmaceuticals in the coming decade will incorporate nitrogen-based heterocycles. The field of medicinal chemistry continues to witness the design and synthesis of numerous novel nitrogen-containing heterocycles, each offering distinct physiological properties and promising applications in drug development. The constant growth in this area underscores the continued exploration and potential of these compounds. These nitrogen-containing heterocycles are usually chiral molecules with their defined 3-D structures. Among early development of metal-free synthesis of chiral molecules, MacMillan's pioneer works on iminium/enamine catalysis of imidazolidinones have inspired ample applications of these molecules in numerous asymmetric transformations. However, the lack of viable functionalities within their structures for extended elaboration has limited a broader synthetic application of the imidazolidinones. With many natural products and pharmaceutical lead melocules possessing a spiroimidazolidinone core, designing a new class of chiral imidazolidinones that possess viable functional groups embedded within their structures will present a substantial synthetic opportunity.

Methods:

- Establish a direct preparation of a chiral spiroimidazolidinone from an amino acid and a *N*-alkylated-*p*-aminophenol.
- Establish an aza-Michael/Michael cascade reaction for the spiroimidazolidinone with a high diastereoselectivity for the overall transformation.
- Establish an overall metal-, and organocatalyst-free one pot sequence.

Results: We have demonstrated a practical and scalable rapid assembly of chiral aza-tricyclic molecules containing six contiguous stereocenters with a moderate to good yield and a universal excellent diastereoselectivity (>20:1 dr). The reaction is highly efficient in a single pot transformation. The use of commercial enantiopure amino acids allows the preparation of enantiopure aza-tricyclic molecules. The aqueous-based reaction is practical and scalable for multi-gram synthesis.

Conclusions: The success of implementing this sub-catalysis concept in the synthesis will pave the way for many efficient chiral catalyst-free preparations of chiral nitrogen-containing heterocycles. The readily accessible 4-imidazolidinones could offer potential physiological properties for the future investigations.

<OMC-02>

Screening and evaluation of novel bioactive peptides for simultaneously down-regulating activities of dipeptidyl peptidase - IV and angiotensin-converting enzyme

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Keywords: SSTY hydrolysate; DPP-IV inhibitory peptides; ACE inhibitory peptides; Type 2 diabetes (T2D); Bioassay-guided fractionation

Background: Chinese soft-shelled turtle (SST) *(Pelodiscus Sinensis)* has a highly valuable economy in Taiwan and Asia according to its multiple healthy benefits in traditional Chinese medicine. The management of diabetes and hypertension could be carried out through control activities of dipeptidyl peptidase-IV (DPP-IV) and angiotensin-converting enzyme (ACE), respectively.
Methods: In the current study, bioassay-guided fractionation using strong cation exchange (SCX) chromatography and reversed-phase high-performance liquid chromatography (RP-HPLC), coupled with liquid chromatography-tandem mass spectrometry (LC-MS/MS) analysis were employed for purifying and identifying the DPP-IV and ACE inhibitory peptides from soft-shelled turtle yolk (SSTY) hydrolysate.
Results: Five novel peptides (LPLF, WLQL, LPSW, VPGLAL, and LVGLPL) were determined, synthesized, and then analyzed in vitro bioassays. Among these peptides, LPSW was evaluated as a potential inhibitor due to its notable activity against both DPP-IV (IC_{50} value of 269.7 μM) and ACE (IC_{50} value of 20.80 μM). Moreover, the understanding of the inhibition mechanism of peptides, their stability against enzymes, and the interaction of the complex of peptide-enzyme was commonly evaluated using specific in vitro assays and molecular docking analysis.
Conclusions: The dual-functional bioactive peptides derived from SSTY hydrolysate could be considered as the functional food ingredients for managing both type 2 diabetes and hypertension.

<OMC-03>

Anti-osteoporosis properties of xanthones from *Garcinia* plants

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Keywords: xanthone, anti-osteoporosis, Rankl fish, mekada, Gacinia

Background: Xanthones, secondary metabolites present in higher plants, fungi, and lichens, have gained attention due to their diverse range of biological and pharmacological activities. With approximately 650 known xanthones identified from natural sources, they exhibit antibacterial, antiviral, antioxidant, and anti-inflammatory properties. These compounds also show inhibitory effects on DNA polymerase, cytotoxicity against cancer cells, and potential as anticancer, antidiabetic, and anti-tumor agents. Recent studies have highlighted their role in promoting bone protection and addressing osteoporosis, making xanthones an exciting area of research with promising therapeutic potential.
Methods: Solvent extraction and column chromatography were employed to extract and isolate xanthones from *Garcinia* plants, specifically *Garcinia cochinchinensis*, *Garcinia vilersiana*, and *Garcinia mangostana*. The isolated compounds underwent chemical modifications via epoxidation, ozonolysis, and acetylation, and their chemical structures were elucidated using FT-IR, UV-Vis, MS, and NMR spectroscopies. Molecular docking and dynamic simulations were utilized for virtual screening of potential anti-osteoporosis molecules, followed by *in vivo* evaluation using a heat-shock-induced Rankl-overexpressing transgenic medaka fish model for osteoporosis. Fish larvae were treated with different doses of the compounds (0.5 -12 μM) for four days, surrounding the induction of osteoporosis phenotype, and subsequent assessment of bone mineralization damage levels was conducted.
Results: From three *Garcinia* species, four xanthone compounds were isolated, while three xanthone derivatives, including two newly synthesized compounds, were obtained through semi-synthesis. Extensive molecular docking analysis of over 400 xanthones resulted in the identification of 20 potential xanthone structures with promising biological activities. Remarkably, *in vivo* tests revealed that xanthones exhibited a significant reduction in bone damage in the fish ($p < 0.0001$) and achieving a bone protection index (I_P) of up to 62.9%.
Conclusions: The results of this study provide compelling evidence that xanthones have the potential to positively impact and preserve bone health.

<OMC-04>

Hydrocinamic acid derivatives as the promising steroid 5α reductase inhibitors

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Keywords: Steroid 5α-reductase type 1 (SRD5A1), non-steroidal inhibitor, caffeic acid amide derivatives, high-performance thin-layer chromatography, human keratinocytes, androgenic alopecia

Background: Steroid 5α-reductase or 3-oxo-steroid-4-ene dehydrogenase is a microsomal and NADPH-dependent membrane-bound enzyme belonging to the oxidoreductase family, which plays a crucial role in steroid metabolism. The overexpression of this enzyme disrupts the equilibrium between testosterone and dihydrotestosterone, leading to the development of androgen-related disorders such as prostate cancer, benign prostatic hyperplasia, hirsutism, and androgenic alopecia. Besides, steroid 5α-reductase type 1 is predominantly localized in human hair follicles on the scalp and plays a vital role in hair growth.
Methods: Caffeic acid derivatives containing amide moieties analogous to those present in finasteride and dutasteride were synthesized through amidation. The series of synthesized hydrocinamic acid derivatives were assessed for their potential as inhibitors of steroid 5α-reductase using an anti-proliferative assay involving the tetrazolium dye, 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyl tetrazolium bromide (MTT). Additionally, an in vitro assay was conducted to evaluate the inhibitory activity of these derivatives on steroid 5α-reductase type 1 (SRD5A1), utilizing human keratinocyte cells (HaCaT) and employing non-radioactive high-performance thin-layer chromatography (HPTLC) for detection.
Results: Caffeic acid N-[3,5-bis(trifluoromethyl)phenyl] amide was a promising non-steroidal suppressor, exhibiting a half-maximal inhibitory concentration (IC_{50}) of 1.44 ± 0.13 μM and relatively low cytotoxicity with an IC_{50} of 29.99 ± 8.69 μM. The compound demonstrated SRD5A1 suppression through mixed mode inhibition, with a Ki value of 2.382 μM based on whole-cell kinetic studies.
Conclusions: Caffeic acid N-[3,5-bis(trifluoromethyl)phenyl] amide shows significant potential for further development as a suppressor of SRD5A1, thereby holding promise as a treatment for androgenic alopecia.

<OMC-05>

Design, synthesis and biological evaluation of novel alkoxy/hydroxyaurones as potent pancreatic inhibitors

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Keywords: aurone, flavonoid, pancreatic lipase inhibition, obesity

Background: Pancreatic lipase–an enzyme responsible for the hydrolysis of dietary fat is a promising target for obesity treatment. Despite the side effects on the gastrointestinal system and its link to liver and kidney injury, orlistat is the only FDA-approval medication for obesity treatment with this mechanism. Aurone is a minor subgroup of flavonoids. Unlike chalcone, flavone and isoflavone, aurone has not been reported as a pancreatic lipase inhibitor. In 2020, our group evaluated *in silico* the binding affinity of 82 published bioactive aurones to human pancreatic lipase. Derivatives of 4,6-dihydroxyaurone and 6-hydroxyaurone possessed significant docking scores (–8.3 to –10.5 kcal/mol). In 2021, Huo et al. synthesized a series of indanone derivatives with excellent inhibition potent (IC_{50} of 0.33 ± 0.02 μM). Structurally, if CH_2 of ring C of indanone skeleton is replaced by oxygen, the skeleton will become aurone. Inspired by our *in silico* results and Hou's work, we designed, synthesized and explored the pancreatic lipase inhibitory activity of aurone derivatives belonging to 3 series–4,6-dihydroxyaurones, 6-hydroxyaurones, and 6-alkoxyaurones.

Methods: 36 aurone derivatives were chemically synthesized. 4,6-Dihydroxyaurone and 6-hydroxyaurone derivatives were prepared by the condensation of substituted benzofuran-3(2H)-ones and benzaldehyde derivatives. 6-Alkoxyaurone derivatives were obtained via ether synthesis of 6-hydroxyaurones and alkyl halides.

Pancreatic lipase inhibition activities were evaluated by the hydrolysis of p-nitrophenyl ester catalyzed by porcine pancreatic lipase. Quercetin and orlistat were used as positive references.

Binding properties were explored by fluorescence quenching assay, molecular docking and molecular dynamics simulation.

Results: Among three series, 6-alkoxyaurone derivatives with long-chain (6–10 carbon) alkoxy substituents showed greater potency. **5g** displayed the most potent activity against pancreatic lipase (IC_{50} of 6.154 ± 1.165 μM), 14-fold higher than quercetin (IC_{50} of 86.98 ± 3.859 μM). Molecular docking and molecular dynamics simulation results clarified the role of long-chain substituent on ring A in interacting with the hydrophobic pocket, pushing the inhibitor molecule closer to the catalytic triad. Fluorescent quenching measurement indicated that aurone derivatives quenched the fluorescence of pancreatic lipase via a static mechanism.

Conclusions: Aurone structures were studied as pancreatic lipase inhibitors for the first time. 6-Alkoxyaurone **5g** with the long chain substitution on ring A displayed the greatest inhibition activity among the tested compounds (IC_{50} of 6.154 μM). The results of this study highlight the potency of aurone–a subgroup of flavonoids in the search for novel natural mimic pancreatic lipase inhibitors.

<OMC-06>

Bridging nature and technology: The synergy of natural products and artificial intelligence

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Keywords: Machine learning, traditional medicine, *Cassia auriculata*, Artificial Intelligence

Background: According to the World Health Organisation (WHO), 80% of the global population relies on traditional medicine, which is primarily based on natural products. Despite the significant advancements in both Eastern traditional knowledge and Western scientific research, a gap exists between the two approaches. Artificial intelligence (AI) is a powerful tool to bridge this gap and merge the strengths of Eastern traditional knowledge and Western scientific methods. AI can be utilised to process and analyse a vast amount of data, and generate predictions. Here, we summarise the work that has been done in our lab in utilising AI to understand the mechanism of different traditional medicine.
Methods: To predict the mechanism of these compounds, ligand-based or proteochemometric prediction models are built using machine learning algorithms such as Random Forest and Parzen-Rosenblatt. Upon validation, compounds from plants such as *Cassia auriculata* and *Symphyocladia latiuscula (Harvey) Yamada* were subjected to the models where potential protein targets for the compounds are predicted. Consequently, these predictions will be validated *in vitro* or *in vivo*.
Results: Protein targets for the compounds have been successfully predicted and validated. For example, in the case of *Cassia auriculata*, AKT2 and PI3K-γ were predicted. The expression of these genes was found to be upregulated in streptozocin-induced rats.
Conclusions: AI is a tool that can be used to understand the mechanism of traditional medicine compounds that have been used for thousands of years. However, data that are used to build these models are still predominantly synthetic compounds, which occupy a different chemical space than natural products. Efforts to collect bioactivity data of natural products should be accelerated to further improve on these prediction models.

<OMC-07>

The α-glucosidase Inhibitory Activity of Avicularin and 4-O-methyl gallic Acid Isolated from *Syzygium myrtifolium* leaves

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Keywords: α-glucosidase, Diabetes, *Syzygium*, Avicularin, 4-O-methyl gallic acid

Background: Diabetes Mellitus is the main cause of death on a global scale. In 2019, there were 463 million people with diabetes, and WHO predicts that by 2030, there will be 578 million. As an antidiabetic agent, α-glucosidase inhibitors are one of the methods employed to reduce the prevalence of diabetes. Diabetes is traditionally treated with *Syzygium* as a primary material, medicine, fruit, ornamental plant, and source of carpentry. This investigation aimed to examine the inhibitory effect of seven species of *Syzygium* against α-glucosidase enzyme using an *in vitro* assay and isolate active substances and ascertain their concentrations in each sample.
Methods: As a solvent, ethanol was used in maceration to extract the substance. Afterward, the extract underwent a series of fractionation techniques, including liquid-liquid extraction, vacuum liquid chromatography, column chromatography, and preparative Thin Layer Chromatography (TLC) for purification and isolation. The compound's structures were elucidated using TLC, UV-Visible spectrophotometry, and nuclear magnetic resonance (NMR) spectroscopy.
Results: Based on concentrations of 100 and 200µg/mL, *Syzygium myrtifolium* exhibited the most significant inhibitory effect, followed by other species of *Syzygium*. The proportion of ethyl acetate had the strongest activity (IC_{50} 0.40 ± 0.02 µg/mL) contrasted to positive control acarbose (IC_{50} 55.39 ± 0.67 g/mL) and quercitrin (IC_{50} 6.47 ± 0.40 µg/mL). Avicularin and 4-O-methyl gallic acid were discovered in the ethyl acetate fraction of *Syzygium myrtifolium* with IC_{50} values of 17.05 ± 0.75 µg/mL and 25.19 ± 0.21 µg/mL, respectively.
Conclusions: As α-glucosidase inhibitory, the results of this study indicate *Syzygium myrtifolium* can be used as a dietary supplement to manage hyperglycemia.

<OMC-08>

In Silico discovery of dual AChE and BACE1 inhibitors for Alzheimer's disease

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Keywords: Alzheimer's disease, QSAR, AChE; BACE1, dual targeted inhibitor, fragment design

Background: Multi-target drug development has become an attractive strategy in discovery of drugs to treat of Alzheimer's disease (AzD). In this study, a rule-based machine learning (ML) approach with classification trees (CT) was applied for the rational design of novel dual-target ac-etylcholinesterase (AChE) and beta-site amyloid-protein precursor cleaving enzyme 1 (BACE1) inhibitors.
Methods: This study proposes a rational drug design method to discover potential dual inhibitors of AChE and BACE1 against Alzheimer's disease (AzD). Classification trees were constructed based on bioactive compounds from the ChEMBL library to develop activity rules for each target. Four AChE inhibition rules and three BACE1 inhibition rules were obtained with good prediction accuracies. By integrating these rules and QSAR models, dual inhibitors were identified from a dataset of bioactive compounds. Docking simulations confirmed their ability to bind with the catalytic domains of both enzymes. Fragment-based drug design was employed to assemble abundant fragments into new dual inhibitors.
Results: Updated data from 3524 compounds with AChE and BACE1 measurements were curated from the ChEMBL database. The best global accuracy of training/external validation for AChE and BACE1 was 0.85/0.80 and 0.83/0.81, respectively. The rules were then applied to screen dual inhibitors from the original databases. Based on the best rules obtained from each classification tree, a set of potential AChE and BACE1 inhibitors were identified, and active fragments were extracted using Murcko-type decomposition analysis. More than 250 novel inhibitors were designed *in silico* based on active fragments and predicted AChE and BACE1 inhibitory activity using consensus QSAR models and docking validations.
Conclusions: The rule-based and ML approach applied in this study may be useful for the *in silico* design and screening of new AChE and BACE1 dual inhibitors against AzD.

SESSION 2. Pharmacology & Clinical Pharmacy

Chairs: **Baohong Jiang, Shanghai Institute of Materia Medica, China**
Varalee Yodsurang, Chulalongkorn University, Thailand
Secretary: **Thuy Huong Le, Ton Duc Thang University, Vietnam**

PCP-01 Drug development based on traditional Chinese medicine
Baohong Jiang, Shanghai Institute of Materia Medica, China

PCP-02 <PCP-02>Emerging concepts in rheumatoid arthritis: the story from proton–-sensing receptors
Wei-Hsin Sun, National Yang Ming Chiao Tung University, Taiwan

PCP-03 Identification of diagnostic biomarkers for ovarian cancer: bench to bedside
Varalee Yodsurang, Chulalongkorn University, Thailand

PCP-04 Study on the antibacterial, antioxidant and hypergycemia-preventive effects of *Lactuca indica* L.-Asteraceae
Tran Thi Thu Hong, Hong Bang International University, Vietnam

PCP-05 Extract from *Hymenopellis radicata* inhibits the growth of 4T1 cancer cells
Nguyen Thi Kim Anh, Industrial University of Ho Chi Minh City, Vietnam

PCP-06 Sulforaphane regulates eNOS activation and NO production via Src-mediated PI3K/Akt signaling in human endothelial EA.hy926 cells
Pham Ngoc Khoi, Pham Ngoc Thach University of Medicine, Vietnam

PCP-07 *In vivo* antidiarrheal effect of Andaliman *(Zanthoxylum acanthopodium dc.)* fruit ethanol extract
Maria Immaculata Iwo, Institut Teknologi Bandung, Indonesia

PCP-08 The antimetastatic effect of insulin-like growth factor binding protein-3 in aerodigestive tract cancers
Thuy Huong Le, Ton Duc Thang University, Vietnam

<PCP-01>

Drug development based on traditional Chinese medicine

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Keywords: *Salviae miltiorrhizae, Panax notoginseng*, salvianolic acid B, ginsenoside Rg1, cardiovascular protection

Background: *Salviae miltiorrhizae* and *Panax notoginseng*, two kinds of the most important traditional herbal medicines, have been widely used in clinic in China for the treatment of cardiovascular diseases.
Methods and Results: Our study contained extract, active compounds, and the combination of active compounds from *Salviae miltiorrhizae* and *Panax notoginsen*g. Salvianolic acids, the water-soluble extract containing salvianolic acid A (SalA), salvianolic acid B (SalB), rosmarinic acid and other phenolic acids, significantly reduced doxorubicin-induced cardiomyopathy in mice, and decreased infarct size, improved left ventricule function function in rat with acute myocardial infarction (AMI). SalA prevented endothelial dysfunction, cardiac remodeling and vascular remodeling in spontaneously hypertensive rats; attenuated aortic aneurysm formation in apolipoprotein E-deficient mice. SalB functioned as a competitive inhibitor of matrix metalloproteinase-9 (MMP-9), attenuated cardiac fibroblast migration, collagen and cytokine secretion, and further efficiently prevented cardiac remodeling. The herb pair, derived from roots of *Salviae miltiorrhizae* and *Panax notoginseng*, has been widely used for improving coronary or cerebral circulation in China. Our study evaluated the cardioprotection of combined SalB and ginsenoside Rg1 (Rg1) against myocardial ischemia/reperfusion injury. SalB-Rg1 combination was found to maintain mitochondrial membrane potential and resist apoptosis and necrosis in H9c2 cell. SalB-Rg1 combination down-regulated myocardial infarct size maintained myocardium structure and cardiac function and improved the viability of cardiac myocytes other than cardiac fibroblasts in rats with ischemia/reperfusion injury.
Conclusions: All of these founding elucidated the cardiovascular protection and the underlying mechanism of the active components from *Salviae miltiorrhizae* and *Panax notoginseng*.

<PCP-02>

Emerging concepts in rheumatoid arthritis: the story from proton-sensing receptors

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Keywords: Rheumatoid arthritis, chronic pain, cytokines, macrophages, proton-sensing receptors

Background: The autoimmune disease rheumatoid arthritis (RA) affects approximately 1% of the global population. RA is characterized by chronic inflammation of synovial joints, then leads to progressive and erosive destruction of bone and cartilage, RA is often associated with ongoing pain and increased pain sensitivity. Chronic pain that comes with RA turns independent, essentially becoming its own disease. Even though gene profiling has been reported and some anti-rheumatic drugs are developed, a significant number (50%) of RA patients, however, do not respond to the current therapies. It still remains a need for advanced understanding of RA pathology and associated pain, in order to seek for novel strategies for preventive, early and curative treatments. The acute phase of pain seems to associate with joint inflammation in early RA. In established RA, the chronic phase of pain could be linked to inflammatory components of neuron-immune interactions and non-inflammatory components. High hydrogen ion concentration (acidosis) found in synovial fluid in RA patients is associated with disease severity. Acidosis signaling acting on proton-sensing receptors may contribute to inflammation and pain.

Methods: We intra-articularly injected complete Freund's adjuvant into mice once a week for 4 weeks to establish mouse RA model. Pain-like behaviors were examined using von Frey filaments for mechanical stimulation and Hargreave's apparatus for thermal stimulation. Blood cytokine levels, macrophages, and microbiota were also examined.

Results: Arthritic mice showed long-lasting bilateral pain hypersensitivity for at least 12 weeks, and long-term joint inflammation, bone erosion, and cartilage damage. Temporal expression of cytokines, tumor necrosis factor α, interleukin 17 and interleukin 6; stage-dependent switch of M1/M2 macrophage polarization; and dysbiosis of gut microbiota regulate RA progression and associated pain sensitivity. Deficiency in either acid-sensing ion channel 3 (ASIC3), transient receptor potential/vanilloid receptor subtype 1 (TRPV1), or T-cell death-associated gene 8 (TDAG8) attenuates RA disease severity and associated RA pain. Deletion of TDAG8 reduces M1 macrophage number, inhibits the increase in cytokines and satellite glial cells, and partly restores gut microbiome. Small compounds blocking TDAG8 expression and function also reduce disease severity and relieve RA pain.

Conclusions: Proton-sensing receptors could be potential targets to therapeutic treatments.

<PCP-03>

Identification of diagnostic biomarkers for ovarian cancer: bench to bedside

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Keywords: Ovarian cancer, Diagnostic biomarkers, GWAS, Chemokines

Background: Ovarian cancer (OC) is the second most common gynecological cancer and the leading cause of death worldwide. Almost 75% of OC are diagnosed in the advanced stage of disease, leading to poor prognosis and high recurrence. Precision medicine has been applied in the management of ovarian cancer to improve patient outcomes and survival. This research focuses on the identification of genetic biomarkers for disease susceptibility as a discovery phase. Regards to current diagnostic tool for OC, serum carbohydrate antigen 125 (CA125) is the most widely used biomarker. However, it demonstrates low sensitivity and specificity for the early detection of OC, e.g., the detection of elevated CA125 levels in non-cancer patients with endometriosis inflammation and patients with other cancer types. The second study revealed the use of the liquid biopsy-based diagnostic biomarkers for OC as a tool for clinical application.
Methods: As a discovery phase, genome-wide association studies (GWAS), using 681 OC cases and 17,492 healthy controls was performed. Functional studies including regulatory feature analysis and electrophoretic mobility shift assay (EMSA) were used to validate the role of single nucleotide polymorphisms (SNPs) in ovarian cancer regulation. As a tool for clinical application, the serum levels of five candidate chemokines were investigated in 98 preoperative women with clinically diagnosed ovarian or adnexal masses using a sandwich enzyme-linked immunosorbent assay (ELISA).
Results: GWAS have identified the genetic variants on chromosome 22q13.1 that are associated with OC risk. Functional studies revealed two regulatory SNPs that affect the binding affinity to nuclear proteins in ovarian cancer cells. The plausible regulatory proteins whose motifs could be affected by the allele changes of these two SNPs were also proposed. For liquid biopsy-based diagnostic biomarkers, CCL20 level could differentiate between benign and early-stage malignancy, with 60.61% sensitivity and 75.44% specificity. Furthermore, CCL20 levels could distinguish endometriotic cysts from OC, whereas CA125 levels could not. Concordant with the serum protein level, the increased mRNA level of CCL20 was observed in ovarian cancers. The logistic regression model integrating CCL20, CA125, and menopause status promoted diagnostic accuracy by increasing the specificity to 91.23%.
Conclusions: GWAS and post-GWAS functional analyses could be utilized for the discovery of diagnostic biomarkers for OC, though, further validation is essential. Our study revealed the potential usefulness of CCL20 level as a liquid biopsy-based biomarker for diagnosing early-stage OC with endometriosis differentiation.

<PCP-04>

Study on the antibacterial, antioxidant and hypergycemia-preventive effects of *Lactuca indica* L.-Asteraceae

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Keywords: *Lactuca indica* L.- Asteraceae, antibacterial, antioxidative, hyperglycemia-preventive effects

Background: Bioactivity-based screening studies have been necessary to find out potential medicinal plants in health promotion and alternative therapy.
Lactuca indica L. Asteraceae (Vietnamese dandelion) are widely used in traditional medicine but there is very little published research on its efficacy in antibacterial, antioxidative effects and diabetic management.
Determining the potential extracts from *Lactuca indica* leaves which possess antibacterial, antioxidative activities and hyperglycemia-preventive effect on experimental studies.
Methods: Aqueous and 45% ethanolic extracts from *Lactuca indica* leaves were evaluated in vitro antibacterial activity (Minimum inhibitory concentration-MIC determination), DPPH (1,2-diphenyl 2-picrylhidrazin) radical-scavenging activity and lipid peroxidative inhibitory activity and the in-vitro assays of α-amylase and α-glucosidase were applied to study on the inhibitory enzyme activities of L. indica leaf extracts (aqueous and 45% ethanol extracts). The blood glucose levels after 30-120 min of mouse oral glucose tolerance test (glucose 2 g/kg BW, per os) were measured to evaluate in vivo effect of these extracts.
Results: *L. indica* leaf ethanoilc extract demonstrated antibacterial and DPPH radical-scavenging activities better than aqueous extract. The MIC value of *L. indica* leaf ethanolic extract on Staphylococcus aureus was 8 times lower than that of aqueous extract. However, *L. indica* leaf aqueous extract had lipid peroxidative inhibitory activity more significant than ethanolic extract.
All of *L. indica* leaf extracts did not present α-amylase inhibitory activity. 45% ethanolic extract exhibited α-glucosidase inhibitory activities (with IC_{50} value of 549.52 µg/ml, equivalent to acarbose) and the modulating effect on blood glucose in oral glucose tolerance test (reducing by 17.2 -22.5%) at the dose equivalent to 2.5 g raw material/kg which were more significant than the aqueous extract (reducing by 11-18%). However, the effect of ethanol *L. indica* leaf extract was less efficient than that of glibenclamide (5 mg/kg).
Conclusions: The revealed results provide a significant effect of L. indica leaves on S. aureus and antioxidant activities for further reseaches, especially markedly lipid peroxidative inhibitory activity of L. indica leaves.
The 45% ethanol *L. indica* leaf extract significantly possessed α-glucosidase inhibitory activity, hyperglycemia-preventing effect and accelerating glucose tolerance.

<PCP-05>

Extract from *Hymenopellis radicata* inhibits the growth of 4T1 cancer cells

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Keywords: Breast cancer, cytotoxicity, ethanol extract, growth inhibition, *Hymenopellis radicata*

Background: Breast cancer is the most common cancer and the leading cause of death in women worldwide. Current drugs to treat breast cancer all have side effects and might lead to drug resistance. Natural chemicals that support cancer treatment including breast cancer and minimize side effects are currently of research interest. Black termite mushroom (*Hymenopellis raditaca*) not only provides nutritional value but also has many valuable biological activities that promise to open up new prospects in medicine. In this study, the cytotoxicity of extracts from black termite mushroom originally grown in China, Thailand, and Vietnam to breast carcinoma cell line 4T1 were investigated.

Methods: Ethanol extraction was used to collect extracts from black termite mushroom. Antioxidant activity was assessed using DPPH method. The concentration $5x10^5$ cell/ml of 4T1 and fibroblast (used as control) was seeded of 200µl per well into 96 well plate. The dilution range of 200, 100, 50, 25, and 12.5 µg/ml was then added to cells. Survival percentage of cells and IC50 were determined 72h after cells exposed to the extracts.

Results: The results of antioxidant analysis showed that all three extracts were able to remove DPPH free radicals, in which the extract of mushroom originated from China gave the highest antioxidant value. At the concentration of 25 µg/ml, alive 4T1 cell number reduced dramatically. The IC50 values of extracts from black termite mushroom originated from China, Thailand, and Vietnam were 17.051 ± 5.751 µg/ml, 19.712 ± 1.336 µg/ml, and 23,361 ± 5,086 µg/ml, respectively. Meanwhile, fibroblast cells were not significantly affected by extract until the 200 µg/ml.

Conclusions: Extract from black termite mushroom effectively inhibits the growth of breast cancer cell line 4T1, which may be a potential medicinal source to support the treatment of breast cancer.

<PCP-06>

Sulforaphane regulates eNOS activation and NO production via Src-mediated PI3K/Akt signaling in human endothelial EA.hy926 cells

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Keywords: Sulforaphane, Src, Akt, eNOS, NO

Background: Sulforaphane is a naturally occurring isothiocyanate that is abundant in many cruciferous vegetables, such as broccoli and cauliflower, and it has been observed to exert numerous biological activities. In the present study, we investigate the effect of sulforaphane on eNOS, a key regulatory enzyme of vascular homeostasis and underlying intracellular pathways, in human endothelial EA.hy926 cells.
Methods: The cell viability was determined by the MTT assay. The NO production was measured using NO-specific fluorescent dyes DAF-2 and DAF-2DA. Protein extraction and a Western blot analysis were performed also.
Results: The results indicate that sulforaphane treatment significantly increases NO production and eNOS phosphorylation in a time- and dose-dependent fashion and also augments Akt phosphorylation in a time- and dose-dependent manner. Meanwhile, pretreatment with LY294002 (a specific PI3K inhibitor) suppresses the phosphorylation of eNOS and NO production. Furthermore, sulforaphane time and dose-dependently induces the phosphorylation of Src kinase, a further upstream regulator of PI3K, while PP2 pretreatment (a specific Src inhibitor) eliminates the increase in phosphorylated Akt, eNOS and the production of NO derived from eNOS.
Conclusions: Overall, the present study uncovers a novel effect of sulforaphane to stimulate eNOS activity in EA.hy926 cells by regulating NO bioavailability. These findings provide clear evidence that sulforaphane regulates eNOS activity and NO bioavailability, suggesting a promising therapeutic candidate to prevent endothelial dysfunction, atherosclerosis and other cardiovascular diseases.

<PCP-07>

In vivo antidiarrheal effect of Andaliman (*Zanthoxylum acanthopodium* dc.) fruit ethanol extract

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Keywords: Antidiarrheal effect, Andaliman fruit extract, oleum ricin

Background: Based on data from the World Health Organization (WHO), diarrhea is the second leading cause of death in toddlers, especially in Africa and Southeast Asia. Traditionally, people treat diarrhea using plant simplicia such as guava leaves and andaliman fruit. Andaliman is a wild plant that grows in North Sumatra and is often used as a spice in cooking. This study aims to examine the antidiarrheal effect of ethanol extract of andaliman fruit in mice with oleum ricini as an inducer of diarrhea.
Methods: The active compounds in andaliman fruit were extracted by maceration using 96% ethanol. The antidiarrheal effect was assessed by determining the frequency of diarrhea, onset of diarrhea, weight of diarrhea and peristaltic index. The two doses of Andaliman fruit ethanol extract (EEBA) tested were 200 and 400 mg/kg body weight of mice.
Results: The yield of andaliman fruit extract obtained was 19.8%. The results of the phytochemical screening showed that EEBA contained tannins, alkaloids and flavonoids. In the anti- diarrheal test, both doses of EEBA significantly ($p<0.01$) inhibited the onset of diarrhea (41.6±9.3 min and 43.8±7.9 min vs. control 19.2±6.1 min). The two EEBA doses did not affect the total stool weight. High-dose EEBA (EEBAT) significantly ($p<0.01$) inhibited stool excretion (9.4 ± 2.1 times) and intestinal peristalsis with a peristaltic index of 36.6 ± 8.5% vs control 66.1 ± 8.5%.
Conclusions: Based on the results of this study, it can be concluded that the ethanol extract of high doses of andaliman fruit (400 mg/kg body weight of mice) has more potent as an anti-diarrheal compared to low doses of EEBA (200 mg/kg body weight of mice).

<PCP-08>

The antimetastatic effect of insulin-like growth factor binding protein-3 in aerodigestive tract cancers

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Keywords: IGFBP-3, Vimentin, metastasis, head and neck squamous carcinoma (HNSCC) and non-small cell lung cancer (NSCLC)

Background: Metastasis is the leading cause of cancer death worldwide, especially aerodigestive tract cancer such as Human head and neck squamous carcinoma (HNSCC) and non-small cell lung cancer (NSCLC). However there are no available therapeutic options to cure tumor invasiveness and metastasis due to cancer complexity. Previous studies have reported the antiproliferative, antiangiogenic and antimetastatic activities of insulin-like growth factor binding protein-3 (IGFBP-3) in both IGF-dependent or -independent manner in various human cell types. Therefore, we investigated the antimetastatic role of IGFBP-3 and its downstream mechanism in aerodigestive tract cancer.
Methods: In this study, to investigate the antimetastatic effect of IGFBP-3 in HNSCC and NSCLC, we utilized several the anti migratory and invasive *in vitro* assays. We also performed the HNSCC orthotopic xenograft model and 4-nitroquinoline-1-oxide (4-NQO)-induced HNSCC model *in vivo*.
Results: Depletion of IGFBP-3 expression enhances the migration and invasion of NSCLC and HNSCC cells *in vitro* and in HNSCC orthotopic mice model, whereas overexpression of IGFBP-3 reverses these invasive phenotypes. The invasion of 4-NQO -induced HNSCC tumors was consistently significantly enhanced in Igfbp3 knockout mice compared with that in wild-type mice. Interestingly, IGFBP-3 regulated the expression of Vimentin, an EMT related marker. We show that IGFBP-3 induces proteasomal degradation and disrupts Vimentin stability by directly binding to Vimentin, and recruiting its association with the E3 ligase FBXL14. Moreover, results show that the C-terminal domain of IGFBP-3 and the head domain of vimentin are critical for their interaction.
Conclusions: These results suggested that IGFBP-3 suppresses Vimentin stability is a promising therapeutic strategy for aerodigestive tract cancer metastasis

SESSION 3. Pharmaceutics & Industrial Pharmacy

Chair: **Chuda Chittasupho ChaingMai University, Thailand**
Secretary: **Quoc-Viet Le, Ton Duc Thang University, Vietnam**

PIP-01 <PIP-01>External stimuli-responsive drug delivery systems for in situ vaccination
Gayong Shim, Soongsil University, Korea

PIP-02 Lysyl oxidase-responsive anchoring nanoparticles for modulation of the tumor immune microenvironment
Jaiwoo Lee, Seoul National University, Korea

PIP-03 Dextran nanoparticle: a versatile nanocarrier for the delivery of therapeutic oligonucleotides
Nguyen Van Hien, Van Lang University, Vietnam

PIP-04 Mesoporous silica particles as versatile platform for immunotherapy
Thanh Loc Nguyen, Sungkyunkwan University, Korea

PIP-05 Jelly loaded with nanogel containing *Mucuna pruriens* seed extract for neuroprotection in Parkinson's disease
Chuda Chittasupho, Chiang Mai University, Thailand

PIP-06 Polydopamine - A versatile biomaterial for drug delivery systems in cancer immunotherapy
Quoc-Viet Le, Ton Duc Thang University, Vietnam

PIP-07 Development of Couette-Taylor crystallizer applied in the pharmaceutical industry
Anh-Tuan Nguyen, Ton Duc Thang University, Vietnam

<PIP-01>

External stimuli-responsive drug delivery systems for in situ vaccination

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Keywords: gene editing, tumor immune microenvironment, transforming growth factor β

Background: Controlling tumor immune microenvironment (TIME) to activate immune cells has been studied as critical for the treatment of cancer. Here, we report that metal lipid hybrid nanoparticles (MLN)-mediated gene editing of transforming growth factor β (TGF-β) can precondition TIME as “immune activated” state for subsequent therapy.
Methods: The MLN was designed to deliver plasmid DNA which express TGF-β single guide RNA and Cas9 protein (pCas-sgTGF), and to convert light to heat. MLN induced photothermal anticancer effect and exposure of calreticulin in B16F10 cancer cells. In vivo gene editing ability of MLN was confirmed with green fluorescence protein (GFP)-stable cells by using a Cas9/GFP sgRNA-expressing plasmid.
Results: MLN-mediated TGF-β editing significantly decreased the secretion level of TGF-β from B16F10 cells. The supernatant of TGF-β-edited B16F10 cells remarkably increased interferon-γ-expressing cytotoxic T cells by reducing regulatory T cell populations. Intratumoral injection of pCas-sgTGF@MLN efficiently inhibited TGF-β expression in B16F10-bearing mice. Subsequent near-infrared (NIR) irradiation completely ablated tumor tissues in pCas-sgTGF@MLN-treated group whereas tumor growth recurred in MLN(+NIR)-treated group without TGF-β editing. Immune profiling of tumor revealed that certain increase of matured dendritic cells, cytotoxic T cells, and interferon-γ expression in pCas-sgTGF@MLN(+NIR)-treated mice. In addition, treatment of pCas-sgTGF@MLN(+NIR) clearly prevent tumor recurrence of rechallenged B16F10 tumor at a distant site, but not of MC38 and EL4 tumors. Protection effect of pCas-sgTGF@MLN(+NIR) was proved with 4T1 lung metastasis model.
Conclusions: These findings suggest the MLN-mediated gene editing of TGF-β switched on “immune activated” tumor microenvironment and consequently potentiated anti-tumor immunity for systemic immune response.

<PIP-02>

Lysyl oxidase-responsive anchoring nanoparticles for modulation of the tumor immune microenvironment

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Keywords: lysyl oxidase, extracellular matrix anchoring, collagen coating, tumor immune microenvironment, immunotherapy

Background: Lysyl oxidase (LOX) plays a critical role in the tumor microenvironment. LOX is responsible for stabilizing the extracellular matrix by facilitating covalent anchoring between collagen molecules. LOX contain a highly conserved C-terminal domain with a copper-binding site and catalyze the oxidative deamination of lysine residues in collagen fibers. In the tumor microenvironment, LOX is overexpressed, leading to increased density and deposition of the extracellular matrix through excessive collagen anchoring. As a result, the LOX-rich tumor microenvironment becomes an attractive target for effective anticancer strategies, distinguishing it from the microenvironment of normal tissue.
Methods: In the current study, we aimed to develop a tumor microenvironment-responsive extracellular matrix-anchoring nanoparticle containing IQ. We coated the surfaces of IQ-loaded polydopamine nanoparticles with collagen (CPN/IQ) to enable them to specifically respond to excessive LOX in the tumor microenvironment. We hypothesized that the collagen on the surfaces of systemically injected CPN/IQ would selectively form LOX-mediated crosslinks with abundant collagen fibers in the tumor microenvironment, eventually creating artificial extracellular matrix near the tumor cells and thereby retain CPN/IQ around the tumor cells to provide stronger anti-cancer efficacy upon near infrared light radiation.
Results: CPN/IQ could form crosslinked structures with the collagen matrix via LOX. In vitro, anchoring of CPN/IQ nanoparticles was observed with LOX-secreting CT26 cells, but this was blocked by a LOX inhibitor. In CT26 tumor-bearing mice, co-administration of nanoparticles plus the LOX inhibitor did not significantly alter the antitumor efficacy among nanoparticles. In the absence of the LOX inhibitor, however, a single administration of CPN/IQ could provide sustained responsiveness to near-infrared irradiation and ablation of primary tumors. In the primary tumor microenvironment, CPN/IQ lowered the Treg cell population but increased the cytotoxic CD3+CD8+ T cell population. In splenic dendritic cells, CPN/IQ treatment significantly increased the CD11c+CD86+ and CD11c+CD80+ cell populations. In a CT26 distant tumor-rechallenge model, CPN/IQ treatment increased the cytotoxic CD3+CD8+ T cell population and provided 100% survival of mice until 64 days.
Conclusions: This study indicates the feasibility of tumor immune microenvironment modulation using LOX-responsive size-transforming nanoparticles. Although we tested the concept in a CT26 cell-derived tumor model, the concept of LOX-responsive collagen matrix- anchoring nanoparticles may be broadly applied to other tumor tissues with LOX-rich tumor microenvironments.

<PIP-03>

Dextran nanoparticle: a versatile nanocarrier for the delivery of therapeutic oligonucleotides

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Keywords: dextran nanoparticle; desolvation; CpG oligonucleotide; CpG adsorption; CpG conjugation

Background: The aim of this study was to prepare and characterize an amino-dextran nanoparticle (aDNP) platform and investigate two loading strategies for unmethylated cytosine-phosphate-guanine (CpG) oligonucleotide.
Methods: aDNP was prepared by desolvation of amino-dextran followed by the chemical crosslinking of amino groups. Size, surface charge, and surface morphology of aDNP was determined by dynamic light scattering and transmission electron microscopy. CpG was either loaded onto aDNP by adsorption (CpG-adsorbed-aDNP) or conjugated to aDNP (CpG-conjugated-aDNP).
Results: In vitro cytokine production by bone marrow-derived dendritic cells (BMDCs) was measured by flow cytometry. aDNPs size and zeta potential could be controlled to produce uniform particles in the size range of 50 to 300 nm, surface charge of -16.5 to +14 mV, and were spherical in shape. Formulation control parameters investigated included the anti-solvent, water-to-anti-solvent ratio, level of amine functionality of dextran, and the molar ratio of glutaraldehyde to amine. aDNP could be lyophilized without additional cryoprotectant. Unloaded cationic aDNP (+13 mV) showed acceptable in vitro hemolysis. Unloaded and CpG-loaded aDNPs showed no cytotoxicity on BMDCs. CpG-loaded nanoparticles stimulated cytokine production by BMDCs, the level of cytokine production was higher for CpG-conjugated-aDNP compared to CpG-absorbed-aDNP.
Conclusions: aDNP is a promising new drug delivery platform as its offers versatility in loading and tuning of particle properties.

<PIP-04>

Mesoporous silica particles as versatile platform for immunotherapy

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Abstract

The regulation of the immune system has emerged as a promising approach for preventing and treating immunity-related diseases, such as cancer, infectious diseases, and autoimmune disorders. However, achieving spatiotemporal delivery of biomolecules to immune cells remains a significant challenge due to drug degradation in vivo and the absence of target moieties. Here, we propose the utilization of mesoporous silica particles as a platform for recruiting and delivering antigens into antigen-presenting cells to modulate immune system activation or suppression for the treatment of cancer and autoimmunity. Mesoporous silica particles possess advantageous characteristics, including large pore volume, surface area, biodegradability, and biocompatibility, enabling effective drug delivery into immune cells without causing significant side effects to the body. By tailoring the biological properties of the payloads loaded into silica particles, we can precisely control the immune response to generate antigen-specific cytotoxic T cells, facilitating immune- mediated eradication of melanoma, or induce antigen-specific regulatory T cells for the prevention and treatment of autoimmune disorders. Through these approaches, we aim to overcome the limitations associated with immune modulation therapies by leveraging the unique properties of mesoporous silica particles as versatile carriers for targeted antigen delivery. These researches hold great potential for the development of novel strategies to enhance immune responses against cancer and provide new avenues for the management of autoimmune diseases.

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<PIP-05>

Jelly loaded with nanogel containing *Mucuna pruriens* seed extract for neuroprotection in Parkinson's disease

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Keywords: *Mucuna pruriens* seed; functional food; Parkinson's disease; levodopa; nanogel

Background: The first line therapy of patients with Parkinson's disease is levodopa (L-dopa) given orally. *Mucuna pruriens* containing natural L-dopa and other phytochemicals was shown to have superior benefits on Parkinson's disease compared with synthetic L-dopa in terms of reducing L-dopa induced dyskinesia.
Methods: The phytochemical constituents of *M. pruriens* seed extract were identified. L-dopa content in the extract was quantified by HPLC analysis. The effects of *M. pruriens* seed extract on cytotoxicity/neuroprotective activity were determined in neuronal cell line (SH-SY5Y cells), kidney cells (HEK293 cells), and Caco-2 cells. Nanogel of *M. pruriens* seed extract was prepared by ionic gelation and characterized by dynamic light scattering. Nanogel was loaded into jelly formulation. The physical, chemical, and microbiological stability of the jelly were observed for 6 months after storage at 4, 30, and 45 °C.
Results: The results show that *M. pruriens* seed extract contains phenolic compounds, flavonoids, tannins, alkaloids, terpenoids, and saponins. The spray-dried *M. pruriens* seed extract contained 5.59 ± 0.21% L-dopa. *M. pruriens* seed extract at 10 ng/mL did not show cytotoxicity against a neuronal cell line (SH-SY5Y cells), kidney cells (HEK293 cells), or Caco-2 cells. Nanogel of *M. pruriens* seed extract had the hydrodynamic diameter, polydispersity index and zeta potential value of 384.53 ± 11.24 nm, 0.38 ± 0.05, and −11.23 ± 1.15 mV, respectively. Nanogel containing extract at the concentration of 10 ng/mL exhibited neuroprotective activity. A jelly formulation containing *M. pruriens* seed-extract nanogel was successfully developed. The prepared jelly exhibited acceptable physical and microbiological stabilities upon 6 months of the stability test. The half-life of natural L-dopa in jelly were 3.2, 0.9, and 0.6 years for storage conditions at 4, 30, and 40 °C, respectively.
Conclusions: The prepared jelly containing natural L-dopa from *M. pruriens* seed extract with the prominent antioxidant activity is a promising option for elderly patients suffering from Parkinson's disease.

<PIP-06>

Polydopamine - A versatile biomaterial for drug delivery systems in cancer immunotherapy

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Keywords: polydopamine, nanoparticle, cancer, immunotherapy, vaccine, in-situ

Background: Polydopamine (PDA), which is synthesized from dopamine, is inspired by the natural polymer melanin. PDA structure bears the number of catechol and hydroxyl groups playing pivotal roles in interaction with other molecules, thus finding their applications as nano-delivery platform for small molecular drugs and proteins. In addition, PDA is able to coat virtually all types of surfaces and equip them with PDA inherence's chemical characterization and functions. Of note, by sharing a similar structure with melanin, PDA is favored in studies as a nano drug delivery system due to their photothermal conversion ability as well as good biocompatibility and biodegradability.
Methods and Results: In our first study, PDA was exploited as a nanoplatform for photothermal therapy. Monoclonal antibody was conjugated on PDA nanoparticles surface to enable them to accumulate in tumor tissue.
In another study, immune modulating drug was encapsulated in the core of PDA nanoparticle due to hydrophobic interaction. The drug-carrying PDA nanoparticle was further tethered with tumor-binding antibody to enhance specific interaction with tumor cells. This system worked as an adjuvant inducing the *in-situ* vaccine effect and sequentially activating the anti-tumor immunity.
PDA was also used as a versatile coating material for DNA microparticles. PDA-coated DNA microparticles was then engineered with T cell-stimulating antibodies and cytokine. The complexed DNA microparticle acted as a potential T cell stimulator both in *in-vitro* and *in-vivo* models.
Conclusions: Compared to other materials, PDA offer many advantages regarding their green synthesis method, biocompatibility, biodegradability, and versatility in drug delivery. PDA-based nanoplatforms and coating material could potentially find useful applications in cancer treatment and other diseases.

<PIP-07>

Development of Couette-Taylor crystallizer applied in the pharmaceutical industry

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Keywords: Pharmaceutical crystallization, nucleation, crystal growth, agglomeration, selective polymorphism, polymorphic phase transformation, purity, morphology, size and size distribution, Couette-Taylor

Background: Improving performance and controlling crystal product properties such as purity, structure, shape, size, and size distribution are critical issues in the pharmaceutical industries because these properties of the product will directly affect human health. The properties of drug crystal are demanded strictly in quality: they must meet pharmacopeia standards through evaluation, licensing, and supervision by reputable US (FDA) or Europe (EMA) agencies before being commercialized on the world market. Therefore, developing the crystallization system to create high-quality crystal products to meet these requirements is very urgent. In the current work, we developed a new crystallizer, a Couette-Taylor crystallizer with a unique Taylor vortex flow, which provides high performance of pharmaceutical crystal products.
Methods: The Couette−Taylor crystallizer (CT) consists of two coaxial cylinders made of stainless steel. The outer cylinder is stationary, while a motor rotates the inner cylinder. For comparison, a conventional Stirred-Tank crystallizer (ST) was designed following a standard Rushton Stirred-Tank crystallizer. The ST crystallizer was manufactured from stainless steel; a turbine impeller and four baffles were installed for adequate mixing. The CT and ST crystallizers were operated at the same operating conditions. Some typical crystal products, including amino acids (l-glutamic acid and l-lysine) and food additives (guanosine 5'mono-phosphate (GMP)), were crystallized in these crystallizers.
Results: The Taylor vortex flow of CT crystallizer significantly impacts the nucleation and crystal growth processes, promoting selective polymorphic crystallization, reducing the polymorphic phase transformation time, and enhancing the productivity and recovery of crystal products. Plus, the crystal size of products induced by the Taylor vortex flow is uniform with a narrow size distribution. Depending on the target production, this crystallizer also can be used flexibly in batch or continuous mode. Furthermore, this crystallizer can be used for various crystallization methods, including cooling and anti-solvent.
Conclusions: This study demonstrates the advantages of the Couette-Taylor crystallizer used in the pharmaceutical industry. The advantage originates from a unique circulating Taylor vortex flow, providing high energy dissipation, high mass transfer at the solid-liquid interface, and inducing a homogeneous supersaturation.

SESSION 4. Pharmacognosy & Natural Products

Chairs: **Seikwan Oh, Ewha Womans University, Korea**
Sornkanok Vimolmangkang, Chulalongkorn University, Thailand
Secretary: **Hien Minh Nguyen, Ton Duc Thang University, Vietnam**

PNP-01 Production of cannabis hairy root and its elicitation for enhancement of triterpenoids
Sornkanok Vimolmangkang, Chulalongkorn University, Thailand

PNP-02 Cytotoxicity activity, metabolite profiling, and isolation compound from crude hexane extract of *Cleome rutidospermae*
Budiman Yasir, Hasanuddin University, Indonesia

PNP-03 Eriodictyol attenuates H_2O_2-induced oxidative damage in human dermal fibroblasts through enhanced capacity of antioxidant machinery
Visarut Buranasudja, Chulalongkorn University, Thailand

PNP-04 Integrative approaches for the identification of suspicious forensic plant specimens from life threatening case in Thailand
Aekkhaluck Intharuksa, Chiang Mai University, Thailand

PNP-05 Evaluation of the antioxidant and anti-tyrosinase effects of *Ochna integerrima* flowers
Hien Minh Nguyen, Ton Duc Thang University, Vietnam

PNP-06 Enantiomer and Anti-Glioma Properties of MMEO Compound (3'-metoxy-3'',4''(Metilendioxy)- 2,5-Epoxilignan-4ol-6one
Yusnita Rifai, Hasanuddin University, Indonesia

PNP-07 Crystal structural analysis of norbelladine 4'-O-methyltransferase
Saw Yu Yu Hnin, University of Toyama, Japan

PNP-08 Melatonin inhibits chondrosarcoma cell proliferation and metastasis by enhancing miR-520f-3p production and suppressing MMP7 expression
Nguyen Bao Tran, China Medical University, Taiwan

PNP-09 Chinese herbal medicine alleviating muscle atrophy in murine myoblasts via the anti-inflammatory effects
Lin-Chu Huang, China Medical University, Taiwan

<PNP-01>

Production of cannabis hairy root and its elicitation for enhancement of triterpenoids

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Keywords: hemp, Cannabis sativa, friedelin, epifriedelanol

Background: Cannabis is a plant that has been used for medicinal purposes for centuries. While the aerial parts of the plant, such as flowers and leaves, have been extensively studied for their cannabinoid content, the root system has been largely neglected. However, recent research has shown that the roots of cannabis have potential as a source of bioactive compounds. In particular, root cultures have been developed to produce compounds such as triterpenoids, which have been shown to have anti-inflammatory and anti-cancer properties. However, the production of such compounds in cannabis is often limited by the availability of plant material. As a result, alternative methods for the production of triterpenoids have been explored, including the use of plant cell cultures. One such culture system is the production of hairy roots, a type of plant cell culture that has the potential to produce high levels of bioactive compounds. Elicitation has been found to be an effective technique for inducing the production of secondary metabolites in plant cells.
Methods: Cannabis hairy roots were induced by *Agrobacterium rhizogenes*. The hairy roots were then exposed to various elicitors and concentrations. The triterpenoids including friedelin and epifriedelanol in the hairy roots and in the soil-grown roots were observed in their presence and amount by using HPTLC and GC techniques.
Results: Hairy roots were successfully established. They grew fast and healthy and contained 1.25-fold higher triterpenoid levels than soil-grown roots. Upon the treatment of methyl jasmonate (MeJA), salicylic acid (SA), yeast extract (YE), and chitosan (CHI), salicylic acid was the most effective elicitor that enhance the level of triterpenoids in the hairy roots much higher than untreated hairy roots.
Conclusions: Overall, the production of cannabis hairy roots represents a promising alternative to traditional methods of cannabis cultivation for the production of valuable triterpenoids friedelin and epifriedelanol. It is easy to harvest and provides a higher content of bioactive compounds by elicitation technique. Further research is needed to explore their potential applications in the pharmaceutical industry. Nevertheless, this approach may provide a new pathway for the development of novel cannabis-based therapeutics that could have significant benefits for patient health and well-being.

<PNP-02>

Cytotoxicity activity, metabolite profiling, and isolation compound from crude hexane extract of *Cleome rutidospermae*

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Keywords: *Cleome rutidospermae*, Stigmasta-5,22-dien-3-ol, Bis(2-Ethylhexyl) esters (DEHP), Cytotoxic

Background: This study isolated the chemical compounds and evaluated the cytotoxic activity of the crude hexane extract of *Cleome rutidospermae* herb (CRH).
Methods: The isolate was purified using silica gel, column chromatography, and preparative thin layer chromatography (PTLC). Furthermore, the structure of the compounds was identified by spectroscopic methods using 1D, 2D NMR, and mass spectrometry. The cytotoxic activity of CRH at a concentration of 20 ug/mL was also tested against MCF-7, A549, KB, KB-VIN, and MDA-MB-231 cancer cells using the **sulforhodamine B** (SRB) method.
Results: The CRH contained compounds of unsaturated fatty acid, saturated fatty acid, lipid, glycerol, ω-3 fatty acid, and cholesterol. Two compounds were obtained from the plant, and their structures were identified as (**1**) Stigmasta-5,22-dien-3-ol (STML) and (**2**) 1,2-Benzene dicarboxylic acid, 1,2-bis (2-Ethylhexyl) esters (DEHP). These compounds were reported in this plant for the first time. In comparison, CRH had % growth inhibition in the proliferation of MCF-7 cells up to 28.1%, with cancer cells A549, KB, KB-VIN, and MDA-MB-231 by >50% Compared to the negative DMSO of 0.20%, while the positive control could inhibit the growth of all cancer cells (100%).
Conclusions: Our findings suggested that crude herb from the plant CRH was the potential for breast cancer treatment.

<PNP-03>

Eriodictyol attenuates H_2O_2-induced oxidative damage in human dermal fibroblasts through enhanced capacity of antioxidant machinery

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Keywords: anti-skin aging, eriodictyol, oxidative stress, antioxidants

Background: Oxidative stress in dermal fibroblasts is strongly correlated with the aging process of the skin. The application of natural compounds that can increase the ability of dermal fibroblasts to counteract oxidative stress is a promising approach to promote skin health and beauty. Eriodictyol is a flavonoid that exerts several pharmacological actions through its antioxidant properties. However, its protective effects on dermal fibroblasts have not yet been investigated. In this study, we aimed to evaluate the beneficial activities of eriodictyol isolated from *Dendrobium ellipsophyllum* against oxidative damage in human dermal fibroblasts. Our findings support the potential utility of eriodictyol for pharmaceutical and cosmeceutical purposes to maintain skin health and beauty.
Methods: BJ cells were used as a model for human fibroblasts and hydrogen peroxide (H_2O_2) were used as an inducer of oxidative stress. To investigate pharmacological effects of eriodictyol, BJ cells were pre-treated with eriodictyol for 24 h then incubated with H_2O_2 for 1 h. Following treatments, cell viability was determined with MTT assay; mode of cell death was characterized with Hoechst 33342/ propidium iodide double staining; cellular redox status was monitored with DCFH-DA-based approach and determination of intracellular GSH; activities and protein expressions of major antioxidant machineries were observed.
Results: Eriodictyol pretreatment significantly prevented necrotic cell death caused by H_2O_2 exposure. In addition, the level of DCFH oxidation was decreased, and that of glutathione was maintained, indicating that the beneficial effects of eriodictyol against H_2O_2 were closely associated with oxidative-stress attenuation. Results from our current study suggested that eriodictyol mediates its antioxidant effects on dermal fibroblasts against H_2O_2 through (i) the direct neutralization of reactive oxygen species; (ii) the enhancement of the activities of H_2O_2-detoxifying enzymes, including catalase and glutathione peroxidase; and (iii) the induction of the expressions of catalase and glutathione peroxidase 1 *via* the activation of the Nrf2 signaling system. These results support the potential application of eriodictyol as an ingredient in skincare products for cosmeceutical and pharmaceutical purposes.
Conclusions: Eriodictyol exerts protective actions against H_2O_2-induced cytotoxicity in dermal fibroblasts by inhibiting oxidative stress. The enhancement of the capacity of antioxidant machinery to detoxify ROS appears to be a principal factor for these beneficial activities of eriodictyol. Our findings suggest that supplementation with eriodictyol could effectively enhance skin viability, promote skin elasticity and increase skin resilience. Altogether, eriodictyol could be a promising candidate for anti-aging purposes in pharmaceutical and cosmeceutical products.

<PNP-04>

Integrative approaches for the identification of suspicious forensic plant specimens from life threatening case in Thailand

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Keywords: Aconitum, Toxicity, Plant Identification, Microscopy, TLC, DNA barcoding

Background: A 37-year-old Thai man accidentally consumed homemade alcoholic herbal maceration intended as a tonic. Approximately one hour after ingestion, he developed symptoms of chest tightness, palpitations, and unconsciousness. His blood pressure was measured at 80/60 mmHg, and his heart rate was 160 beats per minute. He was diagnosed with bidirectional ventricular tachycardia, a life-threatening condition. Preliminary examinations did not reveal any other abnormalities. The physician performed electrical cardioversion, which successfully restored the normal heart rhythm. The cause of the symptoms remains unclear. Therefore, our objective was to identify the life-threatening plant specimens responsible for this toxicity.
Methods: Two pieces of plant specimens were obtained from the patient's relatives. Based on the symptoms and electrocardiographic analysis, reference Aconitum samples were collected for comparison with the suspected specimens. Macroscopy, microscopy, TLC chromatography, and molecular analysis were conducted.
Results: Macroscopic and microscopic analyses revealed that the specimens originated from the roots of the plant, but the species could not be identified. TLC examination results indicated the presence of aconitine in both the unknown specimens and Aconitum samples. For molecular identification using next-generation sequencing, we successfully sequenced all of the samples. Based on BLAST results and phylogenetic analysis, the neighbor-joining tree and the results of BLAST-similarity-based identification confirmed that both suspected specimens originated from the *Aconitum* plant.
Conclusions: The integration of macroscopic, microscopic, TLC, and molecular identification confirmed that the suspicious plant specimens originated from a part of the *Aconitum* plant.

<PNP-05>

Evaluation of the antioxidant and anti-tyrosinase effects of *Ochna integerrima flowers*

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Keywords: Antioxidant, anti-tyrosinase, HaCaT keratinocyte, *Ochna integerrima flowers*

Background: *Ochna integerrima* belongs to the genus *Ochna* which is rich in bioflavonoids, anthranoids, and flavonoids. The whole plant has long been used as traditional remedies. However, the research on the biological activities of *O. integerrima* flowers has been limited. Hence, this study aimed to perform the antioxidant effects on oxidative stress in human epidermal HaCaT keratinocytes. The *in vitro* and *in silico* anti-tyrosinase properties of isolated compounds were also assessed.
Methods: The extracts were tested for antioxidant and tyrosinase inhibition activities using colorimetric assays. Moreover, cytotoxicity effects were evaluated on the viability of the human HaCaT keratinocyte cell line through an MTT assay.
Results: All the extracts from the flowers showed significant antioxidant effects. The EtOAc extract exerted a protective effect on oxidative stress injury induced by H_2O_2 in HaCaT cells. Then, the four isolated compounds including luteolin (1), 6-*γ*,*γ*-Dimethylallylquercetin 7-*O*-*β*-D-glucopyranoside (2), 6-*γ*,*γ*-Dimethylallylkaempferol 7-*O*-*β*-D-glucopyranoside (3), and 6-*γ*,*γ*-Dimethylallyldihydrokaempferol 7-*O*-*β*-D-glucoside (4) were isolated from the EtOAc extract. The antioxidant activity of 1–3 was due to in vitro tyrosinase inhibition with MM-GBSA free binding energies of -78.9, -70.1, and -71.1 kcal mol^{-1}, respectively, compared to 4 with an energy -56.9 kcal mol^{-1} indicated by *in silico* studies.
Conclusions: The findings indicated that *O. integerrima* species is a promising candidate for further antioxidant studies.

<PNP-06>

Enantiomer and Anti-Glioma Properties of MMEO Compound (3'-metoxy- 3'',4''(Metilendioxy)- 2,5-Epoxilignan-4ol-6one

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Keywords: Epoxylignan, Glioma Inhibitor, Ptch, Enantiomer

Background: MMEO (3'-methoxy-3'', 4''-(methylenedioxy)-2, 5-epoxylignan-4'ol-6-one) is an epoxylignan compound synthesized from *Piper nigrum*. This compound has activity inhibiting mRNA expression of protein-patched homolog (Ptch) in human pancreatic cancer cells and may be used for tumor-related diseases. The use of drugs with a single enantiomer has the potential to lead to simpler and more selective pharmacological and pharmacokinetic profiles, as well as increasing the therapeutic index of different metabolic rates of different enantiomers, as well as reducing drug interactions. For example, one enantiomer may be able to provide the therapeutic effect of a drug while another enantiomer is inactive and/or contributes to an undesirable thread of effect, so that the use of a single enantiomer will provide a superior drug and may be preferred over racemic forms of the drug. Compound MMEO blocked the translocation of GLI transcription factors into the nucleus in PANC1. RNA interferences of the Smoothened (Smo) function in PANC1 treated with the compound downregulated the mRNA expression of Ptch.
Methods: In this study, MMEO was enantiomerized by changing its optical rotation using a polarimeter. Then, MMEO and its enantiomers were characterized using four different methods, namely TLC, FT-IR, UV-Vis Spectrophotometry and NMR, then the results were compared. GST-GLI was bound to magnetic beads and was added to MeOH extract of *Piper nigrum* fruits in EtOH solution to see the anti-glioma properties of the plant.
Results: From the H-NMR results, the chemical shift in the form of a multiplet of 6.39-6.78 ppm indicates the presence of ArH benzene, which is in accordance with the literature. The O-CH2-O position has a chemical shift in the form of a singlet at 5.93 ppm, but based on the literature, CH2-O-R has a chemical shift of 3.4 ppm. This is due to the possibility that the MMEO concentration used is dilute, resulting in a shift to a higher δ value. In the hydroxyl group (OH-) which is bonded to the C atom number 4', there is a chemical shift in the form of a singlet of 5.56 ppm, which indicates the presence of an Ar-OH bond. To understand the molecular mechanism underlying the Hh signaling inhibitory effect of DMEO, we checked the expression of a GLI-related gene (Ptch) using real-time quantitative RT-PCR. Compared with the control group, mRNA expression of PANC1 treated with MMEO was slightly down regulated at a concentration of 4.0 μM.
Conclusions: MMEO enantiomers have the same physical properties as MMEO, and have the same optical rotation magnitude, but with different rotation directions. The optical rotation of the MMEO is +32.5148, while the optical rotation of the MMEO enantiomer is -32.5329. With this it can be concluded that the MMEO enantiomer is of type (-) because it has an optical rotation direction counterclockwise. The compound MMEO might be able to modulate Ptch expression in PANC1 due to the inhibition of GLI transcriptional activity.

<PNP-07>

Crystal structural analysis of norbelladine 4'-*O*-methyltransferase

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Keywords: Amaryllidaceae alkaloids, N4'OMT, norbelladine

Background: Norbelladine 4'-*O*-methyltransferase (N4'OMT) is the pivotal enzyme that catalyzes a moderate preference of *meta*-*O*-methylation over *para*-*O*-methylation of norbelladine to generate the common biosynthetic precursor of Amaryllidaceae alkaloids such as haemanthamine, lycorine, galanthamine, and pseudolycorine with a wide range of biochemical and pharmacological properties. Thus, the engineering of this N4'OMT might make an excellent platform to control the regioselectivity of these OMT-forming intermediates for further development of unnatural alkaloid analogs. However, its intimate catalytic mechanism remains unclear. In this presentation, we will discuss the catalytic mechanism of N4'OMT including their regioselectivity of *O*-methylation based on the complex structure of N4'OMT with norbelladine.
Methods: The diffraction data of the co-crystals of N4'OMT and its mutants with norbelladine were collected at 100 K using synchrotron radiation at the Photon Factory (PF) beamline BL-1A. Data were indexed, integrated, and scaled using the XDS package and AIMLESS from CCP4 program suite. The structural model was improved by iterative cycles of manual re-building in COOT and crystallographic refinement in phenix.refine. PyMOL was used for the generation of graphical representations.
Results: The binary or ternary crystal structures of N4'OMT and its variants complexed with *S*-adenosylmethionine (SAM)/*S*-adenosylhomocysteine (SAH) and/or norbelladine were successfully obtained at high resolutions, respectively (~2.0 Å). The complex structures of N4'OMT with norbelladine revealed that norbelladine is located near the methyl group of SAM supported by the catalytic residue Lys158 and chelated with Mg^{2+} ion. Remarkably, norbelladine was accommodated in *meta*- and *para*-orientations, in the structure. Structure-based site-directed mutagenesis revealed that the large-to-small substitutions of N4'OMT Met52 with alanine and serine enhance the *para*-forming-*O*-methylation activities, whereas a small-to-large substitution of N4'OMT Met52 with tryptophan maintains the *meta*-forming-*O*-methylation activities.
Conclusions: The structural based-mutagenesis studies of N4'OMT revealed that the size of the amino acids near the catalytic sites regulated *meta*- and/or *para*-*O*-methylation to generate various biosynthetic intermediates of Amaryllidaceae alkaloids.

<PNP-08>

Melatonin inhibits chondrosarcoma cell proliferation and metastasis by enhancing miR-520f-3p production and suppressing MMP7 expression

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Keywords: chondrosarcoma, melatonin, metastasis, MMP7, proliferation

Background: Chondrosarcoma has a high propensity to metastasize and responds poorly to chemotherapy and radiation treatment. The enzymatic activity of matrix metalloproteinases (MMPs) is very important in chondrosarcoma metastasis. Melatonin exhibits anticarcinogenic activity in many types of cancers by suppressing the expression of certain MMP family members, but this has not yet been clearly determined in chondrosarcoma.
Methods: In this study, we established an *in vitro* and *in vivo* metastasis chondrosarcoma model and investigated the inhibition role of melatonin.
Results: Our study demonstrates that MMP7 plays an essential role in chondrosarcoma cell proliferation, migration, and anoikis resistance. We also found that MMP7 is highly expressed in chondrosarcomas. Our *in vitro* and *in vivo* investigations show that melatonin strongly inhibits chondrosarcoma cell proliferation, migration, and anoikis resistance by directly suppressing MMP7 expression. Melatonin reduced MMP7 synthesis by promoting levels of miR-520f-3p expression, which were downregulated in human chondrosarcoma tissue samples. Pharmacological inhibition of miR-520f-3p markedly reversed the effects of melatonin upon chondrosarcoma proliferation and metastasis.
Conclusions: Our study suggests that melatonin has therapeutic potential for reducing the tumorigenesis and metastatic potential of chondrosarcoma via the miR-520f-3p/MMP7 axis.

<PNP-09>

Chinese herbal medicine alleviating muscle atrophy in murine myoblasts via the anti-inflammatory effects

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Keywords: Sarcopenia, Muscle atrophy, Inflammation, Antcin K, Differentiation

Background: Loss of muscle strength and mass would result in poor quality of life. Sarcopenia is defined as the loss of muscle mass and strength related to age, and severe or pathological skeletal muscle injuries. Muscle atrophy is associated with muscle inflammation and differentiation. Antcin K, an herbal medicine extracted from *Antrodia cinnamomea*, is a unique mushroom in Taiwan that has an anti-inflammatory effect on chronic diseases of metabolism. The aim is to analyze the impact of the anti-inflammatory cytokine Antcin K on the proliferation and differentiation of murine myoblasts.
Methods: This study treated the C2C12 cell line with cardiotoxin (CTX) to induce inflammation. The differentiated myoblasts were treated with CTX for 24 hours to induce inflammation followed by treatment with Antcin K for another 24 hours. The effects of Antcin K on C57BL / 6J mice after CTX-induced muscle injury were analyzed in skeletal muscle tissues by using reverse transcription quantitative polymerase chain reaction (RT-qPCR) and immunohistochemistry (IHC) *in vivo*.
Results: Our *in vitro* results showed that Antcin K reduced CTX-induced cytokine expression and promoted the expression of myogenetic markers. Furthermore, the mice group of Antcin K-treated increased body weight and improved rotarod expression. Our IHC results revealed that Antcin K enhanced myogenesis markers *in vivo.*
Conclusions: Our study suggested that Antcin K appears to be a potential therapeutic herbal medicine due to its anti-inflammatory role in skeletal muscle atrophy.

SESSION 5. Pharmaceutical Biotechnology

Chairs: **Nhat Tu Le, Weill Cornell Medical College, U.S.A**
Yei-Tsung Chen, National Yang Ming Chiao Tung University, Taiwan
Secretary: **Bao Le, Ton Duc Thang University, Vietnam**

PBT-01 Integrated RNA and metabolite profiling reveals the role of TNIK in influenza A virus infection
Nhat-Tu Le, Houston Methodist Research Institute, USA

PBT-02 MicroRNA profiling in Vietnamese nasopharyngeal carcinoma and its application in nasopharyngeal cancer treatment
Thuan Duc Lao, Ho Chi Minh City Open University, Vietnam

PBT-03 Therapeutic potential of targeting Heart Failure (HF)-related microRNAs for HF treatment
Yei-Tsung Chen, National Yang Ming Chiao Tung University, Taiwan

PBT-04 Cannabinoid compounds as tyrosine kinase inhibitors against erb2 for anticancer therapy
Natharin Phattayanon, Payap University, Thailand

PBT-05 *Ganoderma microsporum* immunomodulatory protein acts as a multifunctional broad-spectrum antiviral against SARS-CoV-2 by interfering virus binding to the host cells and spike-mediated cell fusion
Di Ngoc Kha Vo, National Yang Ming Chiao Tung University, Taiwan

<PBT-01>

Integrated RNA and metabolite profiling reveals the role of TNIK in influenza A virus infection

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Background: Influenza A virus (IAV) outbreaks present significant global health risks and understanding the underlying mechanisms of IAV infection pathogenesis is crucial for developing effective strategies to combat these outbreaks. In addition to acute infectious mortality, IAV has been associated with atherogenesis and cardiovascular complications, including acute coronary symptoms and fatal myocardial infarction, highlighting the need for comprehensive investigations. This study investigates the role of TRAF2 and NCK interacting kinase (TNIK) in IAV infection in endothelial cells (ECs).
Methods: We assessed the impact of TNIK depletion in human umbilical vein ECs during IAV infection by integrating RNA-seq and metabolite profiling. This approach allows us to identify mechanisms associated with TNIK and its involvement in IAV infection.
Results: Untargeted metabolomic profiling data demonstrated a significant decrease in nicotinamide adenine dinucleotide (NAD_+) metabolism, indicating an increase in EC senescence during IAV infection. Furthermore, the pentose phosphate pathway and glutathione metabolism exhibited a reduction, suggesting a decline in antioxidant mechanisms during IAV infection. Intriguingly, the depletion of TNIK reversed the effects, indicating that TNIK promotes senescence and reactive oxygen species (ROS)-inducing mechanism. To assess the transcriptional level of TNIK effects on senescence and ROS production, we conducted RNA-seq analysis. However, we did not observe any significant regulation of gene networks following TNIK depletion.
Conclusions: Our data suggest that TNIK plays a crucial role in regulating IAV-induced EC senescence and ROS induction, leading to EC dysfunction. Importantly, these mechanisms appear to be independent of transcriptional rgulation. Further investigation based on proteomic studies is necessary to deepen our understanding of these processes.

<PBT-02>

MicroRNA profiling in Vietnamese nasopharyngeal carcinoma and its application in nasopharyngeal cancer treatment

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Keywords: microRNAs, Nasopharyngeal cancer, case-control

Background: Nasopharyngeal carcinoma (NPC) is a common and malignancies disease in Asia, especially China and Vietnam. Increasing evidences have been indicated that microRNA could the potential candidate for targeted early diagnosis, screening and therapeutic strategies in nasopharyngeal cancer (NPC).

Methods: Total microRNAs were extracted from 100 non-cancerous samples and 93 NPC biopsy samples, then, analyzed by RT-Real time PCR. The relative expression level of miRNA-21, miRNA-155, miRNA-141 in the NPC samples, compared with the controls, was determined by $2^{-\Delta\Delta Ct}$ method. Different bioinformatics tools, including Microtv4, MiRNAMap, miRMap, Mirwalk, Pictar, PITA, TargetScan were applied to predict the targets of these miRAs Interactions among the targets of hsa-miR-21-3p/5p were found by the gene MANIA online tool.

Results: The frequency of miRNA-21, miRNA-155, miRNA-141 detection were 84.95% and 42.00%, 75.27% and 35.00%, 67.74 and 37.00% in NPC biopsies and control samples, respectively. The statistical analysis showed that there was a significant association between the expression of miRNA-21, miRNA-155, miRNA-141 in the NPC samples by increased 7.67, 5.65, and 3.43 time compared with the control group, respectively. Also, it was found that the target genes are involved in vital biological processes in cancer. In detail, a total of 95 targets of miRNA-21, miRNA-155, miRNA-141 were recorded to be associated with NPC.

Conclusions: miRNA-21, miRNA-155, miRNA-141 was upregulated in NPC, thus, it could be speculate that these targets as the promising target for the prognosis and therapy of NPC in Vietnamese population in future.

<PBT-03>

Therapeutic potential of targeting Heart Failure (HF)-related microRNAs for HF treatment

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Keywords: microRNA, heart failure, microRNA-based therapy

Background: Heart failure (HF) is a syndrome that affects 26 million people worldwide, imposing a significant clinical and economic burden on societies. It is a complex syndrome characterized by insufficient cardiac output to meet the metabolic demands of peripheral and major organs. HF is a multifaceted disease resulting from various causes, with hypertension and ischemic diseases being the most common. Despite advancements in neurohormone-based HF therapy, the mortality rate for HF remains high. As a result, the development of next-generation HF therapeutics is an urgent and unmet medical need.

Previous cohort studies, including ours, have revealed distinct profiles of circulating microRNAs in HF patients compared to non-diseased controls. MicroRNAs play a crucial role as post-transcriptional regulators in intracellular signaling pathways, affecting nearly all aspects of cellular processes. The presence of extracellular microRNAs may partially reflect molecular changes within cells and provide valuable insights into the underlying molecular mechanisms of diseases.

We are delighted to share our recent discoveries and present a pipeline for identifying potential microRNAs that can be utilized in the development of downstream microRNA-based HF therapeutics.

Results: The findings of the present study demonstrate the correlations between HF-miRs and neurohormonal signaling. Additionally, the potential therapeutic impact of a microRNA targeting strategy was showcased through its implementation in a mouse model of myocardial infarction.

Conclusions: The presence of dysregulated circulating microRNA entities in peripheral blood provides us with a valuable opportunity to gain insights into the underlying molecular alterations associated with HF pathology. Conducting larger-scale studies will be crucial in elucidating the roles of microRNAs in the pathogenesis of HF and advancing the development of next-generation microRNA-based HF therapeutics.

<PBT-04>

Cannabinoid compounds as tyrosine kinase inhibitors against erb2 for anticancer therapy

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Keywords: cannabinoid, tyrosine kinase, receptor

The ErbB family receptor that transmits signals downstream of its activation is critical for responses in cell division control, proliferation, and differentiation across various cell types in tumors. In numerous malignancies, overexpression of protein receptors in the ErbB family has been associated with a poor prognosis, an increasingly aggressive disease, and a higher risk of disease progression and recurrence. Consequently, novel anticancer agent discovery has been concentrating on the direct pharmacological activities affecting a target protein for the treatment of cancer with specific receptor overexpression. Various distinct bioactive botanical substances have been extensively investigated for their potential pharmacological impact.

Numerous investigations have discovered that cannabinoids have therapeutic effects, primarily in the manner of analgesic, anti-inflammatory, antimicrobial, and anticancer activities. The inhibition of tyrosine kinase domain phosphorylation may be the mechanism through which cannabinoids, especially CBD, CBG, and CBN, suppress intracellular downstream signaling. Cannabinoids (CBD, CBN, and CBG) have been investigated in the present study for their efficacy (50% inhibitory concentration; IC50) in suppressing the survival and inducing program cell death of the ErbB2-overexpressed cancer cell line, SK-OV-3.

The result illustrates the anti-cancer potential of cannabinoids against the SK-OV-3 cell line. The beneficial effects of treatment on cancer cell lines that overexpressed other types of ErbB2 receptor-family proteins are intriguing and warrant further study.

<PBT-05>

Ganoderma microsporum immunomodulatory protein acts as a multifunctional broad-spectrum antiviral against SARS-CoV-2 by interfering virus binding to the host cells and spike-mediated cell fusion

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Keywords: SARS-CoV-2, Fungal immunomodulatory proteins, GMI, Viral binding, Cell fusion, Broad-spectrum antiviral against SARS-CoV-2

Background: Severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) is a highly transmissible coronavirus that has caused over 6 million fatalities. SARS-CoV-2 variants with spike mutations are frequently endowed with a strong capability to escape vaccine-elicited protection. Due to this characteristic, a broad-spectrum inhibitor against SARS-CoV-2 infection is urgently demanded. *Ganoderma microsporum* immunomodulatory protein (GMI) was previously reported to alleviate infection of SARS-CoV-2 through ACE2 downregulation whereas the impact of GMI on virus itself was less understood. Our study aims to determine the effects of GMI on SARS-CoV-2 pseudovirus and the more detailed mechanisms of GMI inhibition against SARS-CoV-2 pseudovirus infection.
Methods: ACE2-overexpressing HEK293T cells (HEK293T/ACE2) and SARS-CoV-2 pseudoviruses carrying spike variants were used to study the effects of GMI in vitro. Infectivity was evaluated by fluorescence microscopy and flow cytometry. Fusion rate mediated by SARS-CoV-2 spike protein was examined with split fluorescent protein /luciferase systems. The interactions of GMI with SARS-CoV-2 pseudovirus and ACE2 were investigated by immunoprecipitation and immunoblotting.
Results: GMI broadly blocked SARS-CoV-2 infection in various cell lines. GMI effectively inhibited the infection of pseudotyped viruses carrying different emerged spike variants, including Delta and Omicron strains, on HEK293T/hACE2 cells. In cell-free virus infection, GMI dominantly impeded the binding of spike-bearing pseudotyped viruses to ACE2-expressing cells. In cell-to-cell fusion model, GMI could efficiently inhibit spike-mediated syncytium without the requirement of ACE2 downregulation.
Conclusions: GMI, an FDA-approved dietary ingredient, acts as a multifunctional broad-spectrum antiviral against SARS-CoV-2 and could become a promising candidate for preventing or treating SARS-CoV-2 associated diseases.

SESSION 6. Pharmaceutical Management & Economics

Chairs: **Van Truyen Le, Former Deputy Minister, Ministry of Health, Vietnam**
Usa Chaikledkaew, Mahidol University, Thailand
Secretary: **Xuan Nam Vo, Ton Duc Thang University, Vietnam**

PME-01 Future challenges of health technology assessment on policy decision making in ASEAN countries: Lesson learnt from Thailand
Usa Chaikledkaew, Mahidol University, Thailand

PME-02 Reducing medication errors: The role of hospital pharmacists in hospital settings
Thuy Thi Thu Ngo, Vinmec Central Park International Hospital, Vietnam

PME-03 Health-related quality of life in patients with COVID-19 in Indonesia: A cross-sectional study
Fajriansyah, Sekolah Tinggi Ilmu Farmasi, Indonesia

PME-04 Economic evaluation of glucosamine in knee osteoarthritis treatments in Vietnam: A preliminary results
Nam Xuan Vo, Ton Duc Thang University, Vietnam

<PME-01>

Future challenges of health technology assessment on policy decision making in ASEAN countries: Lesson learnt from Thailand

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Keywords: Health technology assessment, health policy, policy decision making, ASEAN, Thailand

Introduction: Currently the availability of high-cost health interventions, including pharmaceuticals and medical technologies has been continuously increasing. This has frequently led to an increase in public and patient expectations as well as a limited healthcare resource. Therefore, there is a need for an evidence-based approach to assist policy makers to make decisions on resource allocation under healthcare budget constraint. Health technology assessment (HTA) has been increasingly recognized as one of the most useful tools that can help inform health technology- or health intervention-related policymaking at individual, institutional, national, and international levels in both developed and developing countries.
Objective: The objective of this lecture is to provide the overview and future challenges of health technology assessment on policy decision making in ASEAN countries as well as lesson Learnt about the potential application of HTA in policy decision-making in Thailand.
Materials and Methods: A literature review and other related information was gathered to summarize the contents of the presentation.
Results: HTA information has been increasingly used for making decisions in ASEAN countries especially in the development of Universal Coverage Scheme (UCS). However, there are still challenges. Thailand has been used HTA as a tool to make decision whether drugs should be included in the National List of Essential Medicines (NLEM) as well as whether health intervention and technology should be added in the Health Benefit Package of UCS. Moreover, it has been recently applied for price negotiation, development of clinical practice guidelines, and communication with health professionals.
Conclusion: There were future challenges toward the application of HTA in ASEAN countries to develop the UCS in the future.

<PME-02>

Reducing medication errors: The role of hospital pharmacists in hospital settings

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Keywords: hospital pharmacists, medication errors, medication safety, patients' safety, pharmacists

Background: Medication errors are a significant concern for healthcare professionals and patients alike. These errors can occur at any stage of the medication process, including prescribing, dispensing, and administering medication. Medication errors can lead to severe consequences, including adverse drug reactions, hospitalization, and even death. Therefore, it is crucial to prevent medication errors.

Role of Pharmacists: Pharmacists play a vital role in preventing medication errors. They are medication experts and can identify potential medication errors before they occur. Pharmacists can prevent medication errors by:

1. Reviewing medication orders: Pharmacists review medication orders to ensure that the correct medication, dose, frequency, and route of administration are prescribed. They also check for any potential drug interactions or allergies that the patient may have.
2. Dispensing medication accurately: Pharmacists dispense medication accurately by ensuring that the correct medication and dose are dispensed. They also label the medication correctly with clear instructions for use.
3. Educating patients: Pharmacists educate patients on how to use their medication correctly, including the proper dosage, administration, and any potential side effects.
4. Monitoring patients: Pharmacists monitor patients for any adverse drug reactions or drug interactions. They also work with healthcare providers to adjust medication therapy as needed.
5. Key member of Quality Control team: Root cause analysis, training other healthcare professionals, deploy programs to reduce medication errors.

Conclusions: Pharmacists play a critical role in preventing medication errors. By reviewing medication orders, dispensing medication accurately, educating patients, and monitoring patients, they can help ensure that patients receive safe and effective medication therapy. It is crucial for healthcare providers and patients to work together with pharmacists to prevent medication errors and improve patient outcomes.

<PME-03>

Health-related quality of life in patients with COVID-19 in Indonesia: A cross-sectional study

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Keywords: COVID-19, HRQoL, EQ-5D-5L, Indonesia

Background: In Indonesia, data on Health-Related Quality of Life (HRQoL) during the COVID-19 pandemic are scarce. Therefore, this study aimed to assess and evaluate COVID-19 patients' HRQoL during the COVID-19 pandemic.
Methods: A cross-sectional study with questionnaire completion was adopted, and the participants were patients hospitalized at the Rumah Sakit Darurat COVID-19 (RSDC) Wisma Atlet Indonesia from October to December 2021. Generally, the Bahasa Indonesia version of the Euro Quality of Life 5 Dimension 5 Level (EQ-5D-5L) questionnaire was used to assess HRQoL. Frequency and percentage (dimensional and level), Visual Analogue Scale (VAS) values, and utility index conversion with an Indonesian value set were used in the data analysis. Furthermore, Mann-Whitney independent t-test and Kruskal-Wallis compared the mean EQ-5D-5L score distributions.
Results: In this study, about 154 patients consented to participate as respondents. The greatest and lowest utility index value was 1.000 and 0.311 in 48 and 10 patients at 31.17% and 6.49%, respectively. The average value of the utility index and VAS was 0.762 ±0.23 and 75.00±15.81, respectively. The findings showed that the anxiety/depression component was the most often reported issue among 106 individuals at 68.83%.
Conclusions: COVID-19 affects the health-related quality of life in patients.

<PME-04>

Economic evaluation of glucosamine in knee osteoarthritis treatments in Vietnam: A preliminary Results:

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Keywords: Economic evaluation, Cost-utility analysis, Glucosamine, Knee Osteoarthritis

Background: Osteoarthritis (OA) is the degeneration of cartilage in joints that results in bones rubbing against each other, it causes uncomfortable symptoms such as pain, swelling, stiffness, and can lead to disability. It usually occurs in the elderly and causes a large medical burden. The aim of this study is to evaluate the cost-effectiveness between the standard treatment for osteoarthritis and the standard treatment with added crystalline glucosamine sulfate at various stages.
Methods: The Markov analysis modelling was applied to evaluate the effect of both adding glucosamine compared to standard treatment from a societal perspective during whole patients' lifetimes. Data input was collected by review in previous studies. The outcome was measured in quality-adjusted life years (QALYs), and the incremental cost-effectiveness ratio (ICER) from a societal perspective was applied with 3%-discounted for all cost and outcome. One-way analysis via Tornado diagram was performed to investigate the change of factors in model.
Results: The standard treatment 1 had a cost of 314,758,471 VND and a Quality-Adjusted Life Year (QALY) of 56.9374. In standard treatment 2, which includes the addition of Etoricoxib compared to the standard treatment 1, it was observed that the cost increased when Etoricoxib was introduced (367,478,671 VND). However, at the same time, the QALYs doubled, increasing from 56.9374 to 129.8038. The Incremental Cost-Effectiveness Ratio (ICER) for this comparison was 723,519 VND/QALY. The one-way sensitivity analysis showed that the total arthroplasty and acetaminophen use were factors affected by to ICER the most.
Conclusions: In conclusion, the study provided evidence that the addition of Crystalline Glucosamine Sulfate to the standard treatment, regardless of the stage of osteoarthritis, results in cost-effective outcomes within the acceptable willingness-to-pay threshold in Vietnam. Moreover, the study highlights that early supplementation of Glucosamine leads to a significant reduction in the Incremental Cost-Effectiveness Ratio (ICER) and substantially improves the cost-effectiveness of joint degeneration treatment compared to supplementation at later stages.

SESSION 7. Pharmaceutical Analysis & Quality Control

Chairs: **Duc Tuan Nguyen, University of Medicine and Pharmacy, Vietnam**
JiSuk Lee, Seoul National University, Korea
Secretary: **Truong Huy Nguyen, Ton Duc Thang University, Vietnam**

PAQ-01 <PAQ-01>Triterpene esters from *Uncaria rhynchophylla* hooks are able as new selective inhibitors on HIV-1 protease and their molecular docking study
JiSuk Lee, Seoul National University, Korea

PAQ-02 Structure characterization and immunoregulatory effect of cell wall polysaccharides from Pu-erh tea on RAW264.7 cells by JAK/STAT pathway
Jing Li, Shanghai Normal University, China

PAQ-03 UPLC-QTOF-MS based metabolomics approach for the authentication of *Panax vietnamensis* var *fuscidiscus* and *Panax vietnamensis* var *vietnamensis*
Huy Truong Nguyen, Ton Duc Thang University, Vietnam

PAQ-04 Advancing personalized medicine for tuberculosis with multi-modal metabolomics and lipidomics
Nguyen Phuoc Long, Inje University, Korea

PAQ-05 Potency of bioactive compounds from *Caulerpa racemosa* in handling diabetes-related complications: ADMET properties and molecular docking simulations
Muhammad Aswad, Hasanuddin University, Indonesia

<PAQ-01>

Triterpene esters from *Uncaria rhynchophylla* hooks are able as new selective inhibitors on HIV-1 protease and their molecular docking study

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Keywords: *Uncaria rhynchophylla* hooks, triterpene esters, HIV-1 protease, structure activity relationship, molecular docking

Background: This study aimed to investigate *Uncaria rhynchophylla* hooks that can function as a potential source of HIV-1 protease inhibitors for the development of AIDS therapeutics. In addition, we needed to predict their binding energies with HIV-1 protease and identify their interacting residues by a molecular docking study.
Methods: The isolation process was conducted by bioactivity-directed fractionation and isolation using chromatography -such as silica gel, Sephadex LH-20, and HPLC - and structures were determined by spectroscopy such as MS and NMR. HIV-1 protease activity was assayed by the HPLC method, RNase H of HIV-1 reverse transcriptase (RT) activity was elucidated by the radioactive method, and RNA dependent DNA polymerase (RDDP) of HIV-1 RT activity was tested by the non-radioactive ELISA method. Molecular docking simulations were performed by Discovery Studio 2022 and CDOCKER protocol.
Results: Bioactivity-directed fractionation and isolation from the CH_2Cl_2 extracts of *U. rhynchophylla* were employed to isolate triterpene esters **1**-**8**, which were then characterized: uncarinic acids A-E (**1**-**5**), 3β-hydroxy-27-*p*-*Z*-coumaroyloxyolea-12-en-28-oic acid (**6**), 3β-hydroxy-27-*p*-*E*-coumaroyloxyurs-12-en-28-oic acid (**7**), and 3β-hydroxy-27-*p*-*Z*-coumaroyloxyurs-12-en-28-oic acid (**8**). These triterpene esters **4**-**8** exhibited selective inhibition specifically only of HIV-1 protease, with IC_{50} values between 0.6 and 46.5 μM, but did not show inhibitory effects against RNase H or RDDP of HIV-1 RT. Among them, 3β-hydroxy-27-*p*-*Z*-coumaroyloxyurs-12-en-28-oic acid (**8**) displayed the most potent inhibitory activity (IC_{50} of 0.6 μM). Interestingly, structure and activity relationships revealed that the activities of components possessing an ursane moiety, a *cis* configuration, and a *p*-coumaroyloxy group were more valuable than those of ingredients possessing an oleanane moiety, a *trans* configuration, and a feruloyloxy group. Attractively, molecular docking simulation confirmed the structure-activity relationship and provided insight into the molecular interactions that contribute to the inhibitory activity of these triterpene esters **4**-**8**, exhibiting good binding affinities towards HIV-1 protease, with docking scores of 41-63 kcal/mol.
Conclusions: These findings suggest that these triterpene esters from *U. rhynchophylla* may serve as a new group of selective HIV-1 protease inhibitors and may be useful for the development of combination antiretroviral therapy for AIDS patients.

<PAQ-02>

Structure characterization and immunoregulatory effect of cell wall polysaccharides from Pu-erh tea on RAW264.7 cells by JAK/STAT pathway

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Keywords: cell wall polysaccharide, immunoregulatory, JAK/STAT pathway, Pu-erh tea, structure

Pu-erh tea as a popularity dark tea is due to the attractive flavour, taste, and putative health benefits, including anti-obesity, anti-oxidative, anti-cancerogenic and free radical scavenging. The complex biochemical profile of Pu-erh tea results from microorganism present during the manufacturing process. The critical elements of water-insoluble polysaccharides from Pu-erh tea cell wall could be affected by fermentation process. Here we characterized the structure and evaluated the biological activities of cell wall polysaccharides from different fermentation periods of Pu-erh tea. The pectic fraction extracted by chelator and alkali solutions can activate the production of interleukine-1α and the G-CSF growth factor by RAW 264.7 murine macrophage cells. Moreover, the immunoregulatory mechanism was explored through the signal pathway of JAK-STAT. The pectic fraction polysaccharide was found to upregulate the SOCS1 expression, which inhibited the JAK/STAT signal pathway. In conclusion, Pu-erh tea cell wall polysaccharide was involved to activate downstream signal pathway of JAK/STAT through SOCS1 overexpression and cytokines release leading to immune regulation.

<PAQ-03>

UPLC-QTOF-MS based metabolomics approach for the authentication of *Panax vietnamensis* var *fuscidiscus* and *Panax vietnamensis* var *vietnamensis*

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Keywords: *Panax vietnamensis* var *fuscidiscus*, *Panax vietnamensis* var *vietnamensis*, *Panax vietnamensis*, untargeted metabolomics, authentication

Background: Panax vietnamensis var fuscidiscus (PVF) and Panax vietnamensis var vietnamensis (PVV) are two varieties of Panax vietnamensis and are quite similar in terms of chemical, morphological, and therefore very difficult for consumers to distinguish even though their economic value is very different. The aim of this study was to develop an UPLC-QTOF-MS based metabolomics approach to systematically analyze the microbial differences between PVV and PVF, thereby establishing valuable information for the authentication of these two valuable ginsengs.
Methods: 42 PVF samples and 17 PVV samples were collected in Lai Chau and Quang Nam, respectively. Then, three representative samples from each group were then characterized using ITSr-DNA sequence data. For the UPLC-QTOF-MS analysis, the chromatographic and mass spectrometry separation conditions were optimized to give optimum resolution and good sensitivity for multicomponent analysis. 42 samples (30 PVF and 12 PVV samples) of the training file were used to identify potential ginsenoside discriminant markers using the PLS-DA multivariate statistical model. Next, these indicators are validated using a test set consisting of 17 samples (12 PVF and 5 PVV).
Results: ITSr-DNA sequence data illustrated that the collected samples were true to their origin. Then, the results of PLS-DA multivariate statistical analysis from the UPLC-QTOF-MS analysis showed a clear separation between PVV and PVF groups and suggested thirteen ginsenosides as potential discriminators. Of these differential markers, seven are highly abundant in PVV, including majonoside R2, vina-ginsenoside R13, ginsenoside Rd, ginsenoside Rb1, notoginsenoside Fa, pseudoginsenoside Rs1 and quinquenoside R1. In contrast, the remaining six markers were highly abundant in PVF, including majonoside R1, vina-ginsenoside R2, ginsenoside Rb2, notoginsenoside Fc, notoginsenoside R2, and notoginsenoside R4.
Conclusions: The method developed in our study shows a highly efficient discrimination between PVV and PVF using an untargeted UPLC-QTOF-MS based metabolomics approach, and thus demonstrates a promising authentication application in the quality control of raw materials and preparations derived from PVV and PVF.

<PAQ-04>

Advancing personalized medicine for tuberculosis with multi-modal metabolomics and lipidomics

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Keywords: Tuberculosis, Metabolomics, Lipidomics, Biomarker, Personalized Medicine

Background: Tuberculosis (TB) has remained a global leading cause of morbidity and mortality. Functional omics-based approaches, especially metabolomics and lipidomics, can facilitate the exploration of metabolic and signaling pathways and biomarkers related to TB, both with and without comorbidity. Comprehensive functional omics-based personalized medicine research programs for TB may help improve this disease's diagnosis, treatment, and prevention.
Methods: Herein, I introduce and discuss the main ideas about our multi-modal Liquid Chromatography Mass Spectrometry (LC–MS)-based metabolomics and lipidomics research strategy in discovering and validating novel biomarkers for TB.
Results: The research program is built on four pillars: (1) advancing technology to provide a broader and deeper understanding of the disease and more versatile strategies for data generation, integration, and analysis; (2) conducting generic TB biomarker research to validate proof-of-concept and generate preliminary insights; (3) conducting precision TB biomarker research to noticeably improve the diagnosis and treatment of tuberculosis; and (4) conducting translational omics-based toxicity research to ensure the safe and efficient use of anti-TB therapies. As preliminary results, we discovered and partially validated a number of potential metabolism-centric biomarkers that could be used to improve the diagnosis and treatment monitoring of TB. We also revealed the metabolic changes associated with type 2 diabetes mellitus comorbidity in TB infection.
Conclusions: Current anti-TB management programs have appeared incapable of fully controlling and eradicating TB. Functional omics-based personalized medicine research, although still in its early stages, has the potential to revolutionize TB diagnosis, treatment, and prevention.

<PAQ-05>

Potency of bioactive compounds from *Caulerpa racemosa* in handling diabetes-related complications: ADMET properties and molecular docking simulations

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Keywords: Caulerpa, ADMET, toxicity, docking, diabetes

Background: Diabetes mellitus and its complications are among the primary causes of death and disability. Retinopathy, cardiovascular disease, and neuropathy develop progressively with prolonged hyperglycemia. Finding an effective and secure drug with fewer side effects to handle diabetes-related complications is necessary. Numerous scientists are launching new initiatives to investigate plant sources, which are known to contain a vast array of active agents. An edible marine algae, *Caulerpa racemosa*, was reported to have bioactivities including antidiabetes, anti-inflammatory and neuroprotective.
Methods: The current study was conducted to investigate bioactive compounds from *Caulerpa racemosa* using *in silico* method. 23 compunds were selected to be anticipated their interaction binding mode and interaction energies toward protein target as associated with NF−κB such as TAK1 (7NTI), NIK (4IDV) and MMP−9 (4H3X) using AutoDock Vina integrated with Chimera, while their predicted ADMET were proceeded using web tools such as Swiss-ADME, pkCSM, ADMETLab and Toxtree.
Results: The result indicated that all the compounds were predicted to interact molecularly with amino acids surrounding the binding site of protein targets which were caulerpin, caulersin, racemosin A, racemosin B and racemosin C indicating the most favorable interaction with targets . Predicted pharmakokinetics showed that most of the compounds were lipophilic with poorly solubility while most of them were anticipated as non-toxic agents.
Conclusions: The findings suggested that compounds contained in *Caulerpa racemosa* might potentially to be used in treatment of diabetes-related complications.

SESSION 8. Multimodality Drug Development

Chair: **Byung Hoon Lee, Seoul National University, Korea**
Secretary: **Bich Hang Do, Ton Duc Thang University, Vietnam**

MDD-01 Development of RORα agonists for the treatment of metabolic disorders
Hyeung-geun Park, Seoul National University, Korea

MDD-02 Structure-Activity Relationship (SAR) study of novel nucleoside A2A adenosine receptor antagonist as immune-oncology agents
Lak Shin Jeong, Seoul National University, Korea

MDD-03 Development of therapeutic cancer vaccine against acute myeloid leukemia
Yeonseok Chung, Seoul National University, Korea

MDD-04 Computer-aided drug discovery: From small compounds to protein inhibitors against tyrosine kinase of EGFR for cancer therapy
Kiattawee Choowongkomon, Kasetsart University, Thailand

Acknowledgement
This session is sponsored by Research Institute of Pharmaceutical Sciences of Seoul National University.

<MDD-01>

Development of RORα agonists for the treatment of metabolic disorders

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Keywords: RORα, metabolic disorders, thiourea

Retinoic acid related-receptor orphan receptors α (RORα) has been regarded as critical factors in the regulation of a number of physiological processes. These receptor plays an important role in the development of the cerebellum, lipid and steroid metabolism, hepatic lipid metabolism, homeostasis of cholesterol. Since those physiological functions of RORα can be possibly modulated by exogenous ligands, the discovery of new non-natural ligands may lead to the development of novel therapeutics for human diseases that involve RORα. In 1996, the thiazolidinone type compound CGP52608 were identified as efficient agonists of RORα and showed antiarthritic activity in vivo. As part of our program to develop novel drug-like RORα agonists for the treatment of metabolic disorders, we chose the first non-natural ligand, CGP52608 as a lead compound and attempted to replace the thiazolidin-4-one moiety with the phenyl rings, substituted with various functional groups. In this symposium, we report the synthesis and RORα activity of thiourea derivatives and their biological activities in animal models are also reported for the treatment of metabolic disorders such as fatty liver diseases.

<MDD-02>

Structure-Activity Relationship (SAR) study of novel nucleoside A2A adenosine receptor antagonist as immune-oncology agents

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Keywords: A2A adenosine receptor antagonist, immune-oncology agents, nucleoside, structure-activity relationship

Background: The A2A adenosine receptor (A2AAR) is a subtype of adenosine receptors that has been extensively studied as a target for immune-oncology agents. While modified nucleosides have been developed as A2AAR agonists, only modified purine or heterocyclic compounds have been identified as full antagonists. The ribose moiety, considered crucial for receptor activation, has been targeted for removal to switch from an agonistic to an antagonistic effect.
Methods: Among the synthesized compounds, the most potent one demonstrated high binding affinity (Ki = 7.7 nM) and displayed a full antagonist effect in a cAMP functional assay targeting A2AAR. Additionally, the in vivo anti-cancer effect of this compound was evaluated and showed a significant synergistic effect when combined with the immune checkpoint inhibitor Keytruda. Furthermore, the synthesized compound was used to determine the X-ray co-crystal structure, providing valuable insights into receptor activation.
Results: We revealed the mechanisms of LJ-4378 in enhancing lipolysis and mitochondrial metabolism in brown adipocytes in-vitro, and demonstrated the anti-obesity effects of LJ-4378 in increasing energy expenditure, reducing body weight and fat content, and improving glucose tolerance in high-fat diet-induced obese mouse model in-vivo. Moreover, LJ-4378 induced browning by increasing the expression of brown adipocyte markers and mitochondrial proteins in both brown and white adipose tissues.
Conclusions: Through a combination of SAR study and structural drug design, we successfully discovered novel nucleoside-based A2AAR antagonists. The most potent compound exhibited promising characteristics as a potential immune-oncology agent, as demonstrated by its in vivo anti-cancer efficacy and synergistic effect with Keytruda. Moreover, the elucidation of the X-ray co-crystal structure and the SAR data obtained from this study contribute to a deeper understanding of receptor activation.

<MDD-03>

Development of therapeutic cancer vaccine against acute myeloid leukemia

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Keywords: Acute myeloid leukemia, vaccine, extracellular nanovesicle, NKT cell, CD8 T cell

Acute myeloid leukemia (AML) patients are faced with limited therapeutic options, many of which yield high relapse rates due to resistant clones. Therapeutic vaccines against AML-specific cancer antigens would be effective in repressing residual leukemic cells; however, clonal heterogeneity and low mutational burden of AML make it challenging to define the leukemia-specific antigens. Here we present autologous AML-derived extracellular vesicles loaded with an NKT ligand as an in vivo adjuvant. These autologous vaccines presented endogenously processed class I-restricted cancer epitopes, bypassing the need to identify the cancer antigens when administered autologously. Vaccination with the nanovesicles directly engaged with and induced the activation of iNKT and leukemia-specific $CD8^+$ T cells in AML-bearing hosts, thereby mediating long-term anti-leukemic memory immunity. Human AML-derived extracellular nanovesicles activated iNKT cells from healthy individuals as well as AML patients regardless of disease status. These findings demonstrate that autologous AML-derived extracellular nanovesicles is a promising platform for developing a personalized therapeutic vaccine that efficiently establishes AML-specific long-term immunity without defining cancer antigens.

<MDD-04>

Computer-aided drug discovery: From small compounds to protein inhibitors against tyrosine kinase of EGFR for cancer therapy

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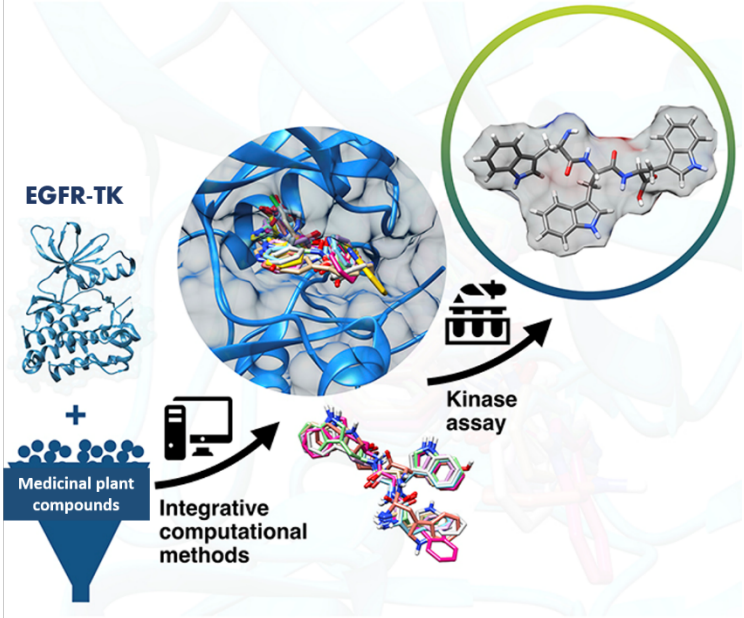
Keywords: epidermal growth factor receptor, cancer, drug

Computational studies are an essential part of research in Biochemistry today. The goal of theoretical investigation of biochemical processes is to gain a deeper insight into the molecular mechanism behind the process of study. It can further be used to predict the results of experiments. Protein Bioinformatics is a useful technique to understand biochemical processes of proteins on various levels including protein modeling, protein docking, and protein molecular dynamics. In our group, we focus on the anticancer targeted protein, the epidermal growth factor receptor (EGFR). This protein plays a crucial role in cellular signaling pathways that regulates key functions, especially proliferation. The EGFR abnormalities have been associated with several types of human cancer. Nowadays, there are cancer-treated drugs that inhibit the activity of tyrosine kinase (TK) domain of EGFR – a signaling part of this protein. However, each drug specifically treats with each cancer type and some tumor patients have resisted to those drugs. A discovery of better new efficient inhibitors is extremely needed. The virtual screening of medicinal plant compound databases against EGFR-TK have been used to discover new inhibitors. These compounds were tested on enzymatic inhibiting assay and non-small cell lung cancer cells, A549.



SESSION 9. YOUNG SCIENTISTS

Chairs: **Thien Y Vu, Ton Duc Thang University, Vietnam**
Duc Toan Pham, Ton Duc Thang University, Vietnam

YC-01 Ligand-based pharmacophore modeling and molecular docking studies of Akt2 inhibitors from marine natural product database
Zenith Putri Dewianti, Bandung Institute of Technology, Indonesia

YC-02 Reviewing the roles of glutathione peroxidase-1 gene on addictive effects induced by cocaine in gene-manipulating mouse model
Duc Toan Pham, Ton Duc Thang University, Vietnam

YC-03 Insight into the structure and physicochemical properties of potent chemokine receptor 5 inhibitors in the discovery of novel Alzheimer's disease drugs
Nur Intan Saidaah Mohamed Yusof, Universiti Teknologi MARA Cawangan Selangor

YC-04 A survey on neuropathic pain medications dosages prescribed by traditional medicine practitioners in diabetic peripheral neuropathy treatment
Nguyen Thi Kim Nhan, University of Medicine and Pharmacy in Ho Chi Minh City, Vietnam

YC-05 Quality of life and associated factors among patients with diabetes mellitus at the Thong Nhat hospital, Viet Nam
Trang Vu Thi, School of Medicine - VNU HCM, Vietnam

YC-06 Association between SLC22A1 gene polymorphisms and the efficacy of tyrosine kinase inhibitors as treatment for chronic myeloid leukemia: A systematic review and meta-analysis
Vu Thi Thuy, Ho Chi Minh University of Technology (HUTECH), Vietnam

YC-07 Phenotypic and molecular assessment on the pharmacological effects of Secang Wood (*Caesalpinia sappan* L.) extract in *Drosophila melanogaster*
Nur Rahma Rumata, Sekolah Tinggi Ilmu Farmasi Makassar, Indonesia

YC-08 Phagocytic activity of trigona honey in male mice (*Mus musculus*) using carbon clearance method
Akbar Awaluddin, Sekolah Tinggi Ilmu Farmasi Makassar, Indonesia

YC-09 Cytotoxic activity of red fruit (*Pandanus conoideus* Lam.) extract on cervical cancer cell line (Hela)
Dewi Purwaningsih, Sekolah Tinggi Ilmu Farmasi Makassar, Indonesia

YC-10 Caffeic acid derivatives inhibit osteoclast functioning, osteoporosis and osteolytic bone metastases
Le Huynh Hoai Thuong, China Medical University, Taiwan

<YC-01>

Ligand-based pharmacophore modeling and molecular docking studies of Akt2 inhibitors from marine natural product database

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Keywords: Ligand-based pharmacophore, virtual screening, docking, Akt2 inhibitors, Marine Natural Product

Background: The mechanism of adaptation of cancer cells nutrient-starved conditions has recently become the center of attention as a possible therapeutic target. The protein kinase Akt is a central signaling molecule within the PI3K/Akt/mTOR pathway. It phosphorylates and regulates the function of many cellular proteins involved in processes that include metabolism, apoptosis, and proliferation. Dysregulated activation of Akt2 has been implicated in several types of cancer. This research aimed to discover potential compounds as Akt2 inhibitors by *in silico* studies. This is part of exploration in studying the cytotoxic activity of Marine Natural Products, especially PANC-1.
Methods: The pharmacophore model of Akt2 was generated and validated to screen the compounds from the comprehensive marine natural products database. Hit compounds from the pharmacophore screening were then subjected to molecular docking. Top five hit compounds were searched for their identity and origin, than visualized for their interaction with Akt2.
Results: AUC 100% of internal and external validation is 0.77 and 0.80, respectively. The root-mean-square deviation (RMSD) of redocking native ligan 4-amino-N-(4-chlorobenzyl)-1-(7H- pyrolo[2,3-D]pyrimidin-4-YL)piperidine-4-carboxamide is 0.7605 Å . Pharmacophore screening yielded 442 hit compounds from a total of 47451 databases. It showed that 216 compounds has lower docking scores and stable binding interaction with Akt2 compared to native ligan. The five best compounds, such as aerophobin 1 (Mediterranean sea), trypargimine (Indonesia, Selat Makassar), 1-carboxytrypargine (Indonesia, Selat Makassar), aerophobin 1 (Italy), and aerophobin 2 (Italy) have 7, 9, 7, 8, and 16 poses interaction with amino acid residues, respectively.
Conclusions: Marine natural product has a promising potential as Akt2 inhibitor. The *in silico* studies provide insights to the development of novel anti-austerity agents and can be continued with molecular dynamics simulations.

<YC-02>

Reviewing the roles of glutathione peroxidase-1 gene on addictive effects induced by cocaine in gene-manipulating mouse model

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Keywords: σ-1 receptor, cocaine, conditioned place preference, glutathione peroxidase-1 gene

Background: Cocaine is an illegal psychostimulant that considered to be highly addictive. The σ-1 receptors in the brain are targets for many psychostimulant drugs such as cocaine and methamphetamine. GPx-1 is an antioxidant enzyme that reported to have neuroprotective effects. In this study, we reviewed our finding about the role of GPx-1 gene on cocaine-induced drug abuse via activation of σ-1 receptor.
Methods: Investigating different effects of cocaine on σ-1 receptor related to drug abuse behaviors using GPx-1 knockout and GPx-1 transgenic mice.
Results: Cocaine significantly increase σ-1 receptor immunoreactivity. The increase of σ-1 receptor parallel with the increase of intracellular signaling pathway mediated oxidative stress damages. GPx-1 gene modification show significant effects on cocaine-induced neurotoxicity via mediating σ-1 receptor function.
Conclusions: In conclusion, our results suggest that GPx-1 gene play an important role on cocaine-induced neurotoxicity via modulating the activation of σ-1 receptor.

<YC-03>

Insight into the structure and physicochemical properties of potent chemokine receptor 5 inhibitors in the discovery of novel Alzheimer's disease drugs

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Keywords: CCR5, Alzheimer's disease, π-π stacking, deep hydrophobic pocket, neuroinflammation, π-π T shaped

Background: In Alzheimer's Disease (AD), chemokines recruit pro-inflammatory mediators and increases the aggregation of both Aβ (amyloid-β) plaque and neurofibrillary tangles (NFTs). Chemokine receptor 5 (CCR5) has been demonstrated to be involved in neuroinflammation and neuroimmunology where its inhibition was shown to enhance memory, plasticity and learning. In this study, compounds that inhibit CCR5 obtained from ChEMBL database were analysed, specifically on whether specific substructures and physicochemical properties are correlated to biological activity.
Methods: Clustering was first performed to group 1,237 compounds into 10 clusters based on the similarities of their structure. Then, molecular docking was performed on 10 compounds that are representative of each cluster. Lastly, Spearman correlation was computed between physicochemical properties and biological activity.
Results: Results showed that potent CCR5 inhibitors tend to: (i) be larger in size (molecular weight of more than 500 g/mol), (ii) bind at the deep hydrophobic pocket, mostly through π-π stacking and (iii) have more than 1 aromatic ring. The larger size may aid in reaching the deep hydrophobic pocket. However, these requirements may lead to the violation of more than 1 Lipinski's Rule of 5.
Conclusions: Future studies should include analyses of the analogues or derivatives of the representative compounds to further expand on the findings here and establish the structure-activity relationship for CCR5 inhibition. This would aid in the development of new AD drugs as drug discovery and development of AD drugs suffer from high attrition.

<YC-04>

A survey on neuropathic pain medications dosages prescribed by traditional medicine practitioners in diabetic peripheral neuropathy treatment

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Keywords: diabetic peripheral neuropathy, traditional medicine, administration and dosage, surveys, and questionnaires

Background: Diabetic peripheral neuropathy (DPN) is one of the most common complications that significantly affects the quality of life in diabetes patients. Recent studies have shown that approximately 20-40% of DPN patients discontinue their neuropathic pain medications, due to two significant factors: insufficient response and adverse effects. Therefore, patients with DPN in Vietnam often choose traditional medicine for ameliorating symptoms. Previous investigations have implicated physicians often lower neuropathic pain medications than recommended. However, in clinical, the prescribing of neuropathic pain medication assigned by Vietnamese traditional medicine physicians have not been surveyed or evaluated.

Objectives: We conducted a survey with the aim of investigating the neuropathic pain medications dosages prescribed by traditional medicine physicians as well as factors influencing the prescribing.

Methods: In this study a cross-sectional analysis was utilized, in which aimed at examining a specific point in time. The survey questionnaire underwent a rigorous development process and was carefully reviewed and approved by the Ethics Committee of the University of Medicine and Pharmacy in Ho Chi Minh City. This comprehensive scrutiny ensured that the questionnaire adhered to ethical guidelines and principles, guaranteeing the protection of participants' rights. Subsequently, this questionnaire was applied at the following hospitals: Binh Duong Traditional Medicine Hospital, Binh Duong Provincial Rehabilitation Hospital, Khanh Hoa Provincial Traditional Medicine and Rehabilitation Hospital, and Can Tho City Traditional Medicine Hospital. The data was recorded in Excel and statistically analysed by using the R programming language. The dosage levels of neuropathic pain medications, as well as the various factors that influenced the indication of these medications, were analyzed and reported with frequency distributions and percentages. To assess the correlation between the indicated dosage and relevant factors, a multivariate linear regression model was employed to identify significant predictors that had a substantial impact on the dosage prescribed.

Results: Of the total 63 doctors, the findings revealed that 53 doctors (84.13%) reported using pregabalin, 58 doctors (92.07%) used gabapentin, 23 doctors (36.51%) employed amitriptyline, and 14 doctors (22.22%) prescribed duloxetine in their clinical practice for the treatment of neuropathic pain.

The results showed that the initial, maintenance, and maximum doses commonly used for pregabalin were 75-150 mg/day, gabapentin were 300-600 mg/day, amitriptyline were 25-50 mg/day, and duloxetine were 30-60 mg/day.

The factors of age, gender, educational level, years of professional experience, and years since university graduation do not have a significant impact on determining the initial, maximum, and maintenance dosage of pregabalin, amitriptyline, and duloxetine. The number of years since university graduation influenced the maximum and maintenance doses of gabapentin ($p<0.05$).

Reasons for medication discontinuation including: efficient response from traditional medicine interventions (73.58% for pregabalin, 70.70% for gabapentin, 43.48% for amitriptyline, 50% for duloxetine); side effects (62.60% for pregabalin, 56.9% for gabapentin, 73.91% for amitriptyline, 50% for duloxetine); and inadequate desired effectiveness (94.34% for pregabalin, 41.38% for gabapentin, 52.17% for amitriptyline, 42.86% for duloxetine).

The utilization of low-dose medication is justified by its ability to achieve therapeutic efficacy even at reduced dosages (60.38% for pregabalin, 56.90% for gabapentin, 65.22% for amitriptyline, 65.29% for duloxetine); traditional medicine modalities have demonstrated significant effectiveness in improving patient outcomes (60.38% for pregabalin, 56.90% for gabapentin, 47.83% for amitriptyline, 50% for duloxetine); side effects-induced intolerance in patients (52.83% for pregabalin, 48.28% for gabapentin, 39.13% for amitriptyline, 50% for duloxetine).

Conclusions: Most traditional Vietnamese physicians lower doses of neuropathic pain medication for diabetic peripheral neuropathy than the recommended guidelines. The primary reason for treatment discontinuation is that the observed inadequate efficacy, while the physicians have not prescribed the maximum recommended dosage. Therefore, it is essential to implement measures to encourage physicians to prescribe the correct dosage according to the recommendations before concluding the failure in treatment. Furthermore, traditional medicine therapy have shown significant efficacy in promoting substantial improvements. This suggests the promising benefits integrating traditional medicine into diabetic peripheral neuropathy treatment in Vietnam, resulting in the enhance therapeutic efficacy compared to using individual conventional medicine.

<YC-05>

Quality of life and associated factors among patients with diabetes mellitus at the Thong Nhat hospital, Viet Nam

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Keywords: Quality of life, type 2 diabetes mellitus, AsianDQOL

Background: Health-related quality of life (HRQOL) has been an important outcome measure for type 2 diabetes mellitus (T2DM) management, which requires a combination of pharmacotherapy and self-management. This study aimed to assess HRQOL and its associated factors among patients with T2DM at Thong Nhat hospital, Vietnam.
Methods: We conducted a cross-sectional study on 418 patients with T2DM at Thong Nhat hospital, Ho Chi Minh City. The Asian Diabetes Quality of life questionnaire (AsianDQOL) was employed to evaluate HRQOL via face-to-face surveys.To compare HRQOL scores between the participants with different characteristics, one-way ANOVA test, independent t-test were performed. Linear regression was applied to identify the factors associated with HRQOL scores.
Results: The result showed that dual therapy was the most commonly used regimen (43.51%). Metformin, DPP-4i and SU were most commonly used (91.37%, 52.30%, and 48.44%, respectively). The mean score of overall HRQOL was 77.19 ± 6.67, in which mean scores for the financial, memory and cognition, physical health, diet and eating habits, inter-personal relationship were 96.90 ± 7.68, 86.58 ± 10.85, 78.38 ± 17.71, 70.58 ± 8.90, and 45.36 ± 16.80, respectively. Linear regression analysis indicated that the HRQOL scores was lower in patients experiencing hypoglycemia once/few months (b= - 2.640, 95% CI = -3.841; -1.438, $p < 0.001$) or ≥ once/week (b = -5.030, 95% CI = - 8.124; -1.936, $p = 0.001$) compared to those without that event. Insulin-treated patients and higher level of fasting blood glucose had lower HRQOL scores with (b = -2.139, 95% CI = -3.741; -0.537, $p = 0.009$), (b=-0.473, 95% CI = -0.929; -0.017, $p = 0.042$), respectively. In contrast, patients doing physical activities had higher QOL score than patients who did not (b = 2.822, 95% CI = 1.464; 4.180, $p < 0.001$).
Conclusions: Among T2DM outpatients in Thong Nhat hospital, the lowest HRQOL score was in the "inter-personal relationship" aspect and the highest was in the "finance" aspect. Physical exercise, adequate glycemic control as well as consulting using drugs could improve diabetic patients' HRQOL.

<YC-06>

Association between SLC22A1 gene polymorphisms and the efficacy of tyrosine kinase inhibitors as treatment for chronic myeloid leukemia: A systematic review and meta-analysis

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Keywords: chronic myeloid leukemia; meta-analysis; tyrosine kinase inhibitor; systematic review; SLC22A1 polymorphism

Background: A systematic review and meta-analysis were conducted to assess the effects of polymorphisms of solute carrier family 22-member 1 (SLC22A1) gene on the effectiveness of tyrosine kinase inhibitors (TKI) as treatment for chronic myeloid leukemia (CML).
Methods: A systematic search of articles published up to October 2022 was performed on PubMed, Cochrane Library, Embase, and Web of Science. The search was based on the main keywords relevant to chronic myeloid leukemia, tyrosine kinase inhibitors, and SLC22A1 gene polymorphisms. A meta-analysis was carried out, and a fixed- effects or random-effects model was used to estimate the pooled odds ratio (OR) with a 95% confidence interval (CI) depending on the heterogeneity between studies. Both pool analyses, heterogeneity between studies assessment, publication bias evaluation, and sensitivity analysis were performed using R software.
Results: Out of 983 records, 13 eligible studies were included in the meta-analysis, with therapeutic effects outcomes including complete cytogenetic response and major molecular response (MMR). The studies evaluated a number of SNPs in the SLC22A1 gene in relation to the therapeutic effects of imatinib on CML patients. Pooled analyses revealed an association between the dominant (AA+AG vs. GG, OR: 0.61, 95% CI: 0.46–0.82, p < 0.01) or homozygote (AG vs. GG, OR: 0.46, 95% CI: 0.23–0.94, p=0,033) model of the SNP 1222 G>A and lower MMR rates. The results of the subgroup analyses showed that the association was only significant for the Asian race. A relationship between achieving reduced MMR rates and the SNP 408 C>G was also identified in all five genetic models (CG+GG vs. CC, OR: 0.52, 95% CI: 0.38–0.72, p < 0.01; GG vs. CG+CC, OR: 0.40, 95% CI: 0.21–0.77, p = < 0.01; GG vs. CC, OR: 0.33, 95% CI: 0.17–0.64, p = 0.001; CG vs. CC, OR: 0.61, 95% CI: 0.38–0.97, p = 0.036; and G vs. C, OR: 0.53, 95% CI: 0.41–0.70, p < 0.01).
Conclusion: Meta-analysis showed that the 1222 G>A and 480 C>G variants of the SLC22A1 gene were associated with decreased imatinib response in the treatment of chronic myeloid leukemia. The results support the evidence that the SLC22A1 variants can be used as signals to predict imatinib's effectiveness in chronic myeloid leukemia treatment, particularly in Asian patients.

<YC-07>

Phenotypic and molecular assessment on the pharmacological effects of Secang Wood (*Caesalpinia sappan* L.) extract in *Drosophila melanogaster*

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Keywords: Anti-aging; Secang; Caesalpinia sappan L.; D. melanogaster; in vivo

Background: Secang, a natural product, possesses a wide range of pharmacological activities, including antioxidant, antibacterial, and anti-inflammatory effects. Its therapeutic potential in improving aging conditions has been investigated due to its ability to inhibit free radicals and melanogenesis. However, most studies have been limited to in vitro conditions. To bridge this gap, we conducted in vivo experiments using the fruit fly Drosophila melanogaster to investigate the anti-aging activities and biological significance of Secang.
Methods: Various parameters were assessed through different assays, including Secang toxicity assay, fly survival, locomotor response to Secang treatment (with or without cigarette smoke), trypan blue staining, larval crawling assays, and gene expression analysis.
Results: Our data revealed no significant differences in toxicity and locomotor tests across various concentrations of Secang. D. melanogaster tolerated concentrations of 0.4%, 0.08%, 0.016%, and 0.0032%, indicating its safety without adversely affecting locomotor function. Furthermore, Secang at a concentration of 0.08% extended the lifespan of D. melanogaster exposed to cigarette smoke while reversing the negative effects of smoke exposure on gut cell viability and larval locomotor activity. Interestingly, Secang increased the expression levels of sod, cat, and srl genes. These findings suggest that Secang administration is safe for D. melanogaster and may have potential benefits for longevity and locomotor function.
Conclusions: The results support the idea that Secang possesses in vivo antioxidant properties and may serve as a promising pharmacological agent. However, further studies are needed to explore its potential applications in human health and disease management, particularly in the context of anti-aging.

<YC-08>

Phagocytic Activity of Trigona Honey In Male Mice (Mus musculus) Using Carbon Clearance Method

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Keywords: Phagocytosis, Immunostimulant, Trigona Honey, Carbon Clearance Method

Background: Improvement of host immunity is achievable through the use of immunostimulant. Trigona honey is one of the ingredients whose use is believed to improvement immunity due to its high content of flavonoid compounds. The objective of the study was to determine the effect of trigona honey on phagocytic activity in male mice using carbon clearance method based on the value of the phagocytosis constant (K).
Methods: Mice were divided into 5 groups as follow: the negative control group was given by aquadest only, the positive control was given by Stimuno®, and the treatment groups were given by 0,3 g/kg BW, 1,5 g/kg BW and 7,5 g/kg BW, respectively, of trigona honey. The treatment was administered orally for 6 days. On the 7th day the mice were injected intravenously of carbon.
Results: The treatments of 0,3 g/kg BW, 1,5 g/kg BW dan 7,5 g/kg BW of trigona honey significantly improvement phagocytic activity ($P < 0.05$).
Conclusions: The results showed that trigona honey could improve phagocytic activity in male mice (Mus musculus), with the best results at a dose of 1,5 g /kg BW.

<YC-09>

Cytotoxic activity of red fruit (*Pandanus conoideus* Lam.) extract on cervical cancer cell line (Hela)

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Keywords: Red Fruit, Hela Cell, MTT assay, Cytotoxic, IC_{50}

Background: Indonesia is one of the mega-biodiversity countries, with many plant species that are useful as medicine. Red Fruit (*Pandanus conoideus* Lam), found in Manokwari, West Papua, is empirically believed to have numerous health benefits such as natural antioxidant and anticancer, due to having a huge number of bioactive compounds, especially carotenoids. The high antioxidant content in red fruit is able to ward off and break free radicals that carry carcinogen compounds. Cervical cancer continues to be listed among the top gynecologic cancers worldwide. Research continues to look for therapies and the current treatment approach is to use natural compounds from plants. This study aimed to determine of red fruit extract that extracted using solvents with different polarity levels (acetone, chloroform, and n-hexane) is able to inhibit the growth of the Hela cell line with varying concentration levels.
Methods: Red fruit extracted using 3 different solvents (acetone, chloroform, n-hexane) with macerator-magnetic stirrer. The experiment used 4 dosages of each Red Fruit extract, 31,25 µg/mL, 62,5 µg/mL, 125 µg/mL, and 250 µg/mL, exposed to Hela cell line and Doxorubicin was used as a positive control. Cytotoxic activities were evaluated by MTT (3-[4,5- dimethylthiazol-2-yl]-2,5 diphenyl tetrazolium bromide) Assay, while Inhibitory Concentration 50 (IC_{50}) was determined through regression-correlation analysis.
Results: The results of the cytotoxic activity of the three types of red fruit extracts on hela cells showed IC_{50} values respectively, acetone extract 72,6 µg/mL, chloroform extract 114,3 µg/mL and n-hexane extract 120,77 µg/mL.
Conclusions: The result showed that the higher the concentration of red fruit extract, the lower the percentage of viable Hela cell and the lowest IC_{50} value was acetone extract which was included in the moderate cytotoxic category.

<YC-10>

Caffeic acid derivatives inhibit osteoclast functioning, osteoporosis and osteolytic bone metastases

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Keywords: MPMCA, Lung cancer, Breast cancer, Osteoclastogenesis, Osteoporosis

Background: Osteoclast activity is fundamental in the disease processes of osteoporosis and osteolytic bone metastasis. Pharmacological agents that treat these diseases are based on the inhibition of osteoclast activity. However, important disadvantages of existing antiresorptive and bone anabolic therapies are their common and rare adverse effects, which limit their long-term treatment in patients, many of whom are elderly and/or have multimorbidities. We are developing a novel compound, MPMCA (a derivative of caffeic acid), which effectively inhibited osteoclast formation and induced mature osteoclast apoptosis in our preliminary studies. Our proposed research aims to determine the underlying mechanisms of this inhibitory activity and examine how MPMCA inhibits osteoporosis.
Methods: In this study, we applied tartrate-resistant acid phosphatase (TRAP) staining to perform osteoclast differentiation exposed to MPMCA treatment. Gene Expression Omnibus (GEO) (GSE21639 and GSE93639) and Gene Expression Profiling Interactive Analysis (GEPIA) databases to asset the gene expression during osteoclast differentiation and cancer progression.
Results: As mentioned above, MPMCA impeded osteoclastogenesis and stimulated mature osteoclast apoptosis. Our preliminary studies also found that MPMCA inhibits tumor necrosis factor alpha (TNF-α) expression in lung and breast cancer cells; production of this osteoclastogenic cytokine is necessary for osteolytic lung and breast cancer metastases. This research plan will therefore examine whether MPMCA inhibits osteoporosis and osteolytic bone metastasis in cellular and preclinical experiments.
Conclusions: It is hoped that the results from this research will encourage the development of a new way of treating osteoporosis and osteolytic bone metastases.

POSTER PRESENTATIONS

Organic & Medicinal Chemistry

PP-01 A machine-learning model to predict P-gp inhibitors
Du Thien Nguyen, School of Medicine - VNU HCM, Vietnam

PP-02 Discovery of natural interleukin 36γ small molecule inhibitors by pharmacophore screening, docking analysis, ADMET prediction, and molecular dynamics simulations
Tuan Le Anh Nguyen, Lac Hong University, Vietnam

PP-03 Synthesis, physiochemical characterization, and bioactivity of *α*-mangostin integrated cellulose hydrogel
Lich Hoang Phan, Ton Duc Thang University, Vietnam

PP-04 Synthesis and characterization of isosorbide-based biodegradable poly(*β*-amino ester) for drug delivery applications
Khanh Vi Nguyen, Ton Duc Thang University, Vietnam

PP-05 Synthesis and surfactant-mediated modification of nanocrystalline cellulose for *α*-mangostin delivery
Kim Ngan Luu, Ton Duc Thang University, Vietnam

PP-06 Chemical constituents and antioxidant evaluation of *Ochna integerrima* (Lour.) Merr. stem
Khanh Phuc Nguyen, Ton Duc Thang University, Vietnam

PP-07 Polycation-modified Fe(III)-MOF loaded with methotrexate and Pt(IV) prodrug for synergistic anticancer therapy
Viet-Phuong Bui, Vietnam National University, Vietnam

PP-08 Transmembrane amyloid β-peptide structures: In silico study
Son Tung Ngo, Ton Duc Thang University, Vietnam

Pharmacology & Clinical Pharmacy

PP-09 Anti-cancer effects of indirubin derivative against acute myeloid leukemia
Keon Wook Kang, Seoul National University, Korea

PP-10 Evaluate the efficacy of early use of remdesivir among patients with COVID-19
Dang Thi Huynh Nhu, Ton Duc Thang University, Vietnam

PP-11 Intervention of pill card to improve medication adherence among HIV patients at one primary health care in Bandung Indonesia
Pratiwi Wikaningtyas, Institut Teknologi Bandung, Indonesia

PP-12 Blood pressure lowering effect of Jamaica cherry (Muntingia calabura L.) leaves and its fraction
Afrillia Nuryanti Garmana, Institut Teknologi Bandung, Indonesia

PP-13 Inappropriate prescribing of antipsychotic drugs in elderly patients at a psychiatry hospital in Viet Nam using stop/start criteria and APID index
Tran Thi Huong, Lac Hong University, Viet Nam

PP-14 Depression status among type 2 diabetes patients in Gia Dinh people's hospital

Trinh Van Luan, Ton Duc Thang University, Vietnam

Pharmaceutics & Industrial Pharmacy

PP-15 Preparation of cough lozenges from the Vietnamese traditional remedy “Bach Bo Bo Phe”
Nguyen Phuoc Vinh, School of Medicine - VNU HCM, Vietnam

PP-16 Formulation of mouthwash solution containing microemulsion of *Ocimum gratissimum* essential oil for antibacterial action in the oral cavity
Dang Lan Vy, University of Medicine and Pharmacy at Ho Chi Minh City, Vietnam

PP-17 Zwitterionic cyclodextrin nanocarrier for tumor targeted drug delivery
Dae-Duk Kim, Seoul National University, South Korea

PP-18 Development of nanoformulation containing fluconazole and ibuprofen to tackle the *Candidiasis*’s fluconazole-resistance phenomenon
Xuan-Phuong Thi Ngo, School of Medicine - VNU HCM, Vietnam

PP-19 The application of ion-exchanging resin in fexofenadine orally disintegratting tablet formulation
Quoc Thai Nguyen, Ton Duc Thang University, Vietnam

PP-20 Tolerogenic nanovaccine formulation in treatment of automatic disease
Thi Mai Phuong Nguyen, Ton Duc Thang University, Vietnam

PP-21 Formulation and in vitro evaluation of film-coated tablets contaning sitagliptin and metformin hydrochloride 50/1000 mg
Thanh Phuong Tran, Ton Duc Thang University, Vietnam

Pharmacognosy & Natural Products

PP-22 The non-saponin fraction of Korean Red Ginseng suppresses muscle loss by maintaining immune homeostasis in old mice
Boo-Yong Lee, CHA University, Korea

PP-23 Optimize steam distillation extraction and make care-hair gel with *Citrus maxima* peel essential oil
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PP-25 Chemical constituents of *Radix Gomphandrae molis*
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PP-26 Morphine dependence is attenuated by the treatment of *Panax ginseng* and *Polygalae radix* combination treatment in mice
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PP-27 *α*-Glucosidase inhibitory potential of *Homonoia riparia*: implications for diabetes mellitus intervention
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PP-28 The anti-inflammatory activity of the extracts and compounds isolated from stems and leaves of *Dichroa febrifuga* Lour.
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Rika Hartati, Bandung Institute of Technology, Indonesia

PP-33 Botanical characteristics, DNA barcode, preliminary screening of phytochemical constituents of *Paederia foetida* Linn., Rubiaceae
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PP-34 α-glucosidase inhibitors from the stems of *Knema globularia*
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PP-35 A olean-type triterpenoid and a sterol isolated from the roots of *Parietaria debilis* G.Forst. Urticaceae
Lieu Lam Khanh, Ton Duc Thang University, Vietnam

PP-36 Investigation of anti-inflammatory activity from extract and isolated compound in the aerial part of *Houttuynia cordata*
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PP-39 The potential application of black shallot, a novel product of shallot (*Allium ascalonicum*), in terms of protection against alcoholic related liver injury
Tinh-Binh Hua, Ton Duc Thang University, Vietnam

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PP-41 Hopan-type triterpenoids from the thallus of lichen *Parmotrema tinctorum* (Despr. ex Nyl.) Hale
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PP-44 Determination of vitamin C in multivitamin gummy candies for children by HPLC - PDA method
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PP-50 Design and evaluating the efficacy of novel antibodies enhancing binding on CTLA-4 and PD-1 immune checkpoints
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PP-51 Investigation of alpha-glucosidase inhibitory effect of aqueous extract from flora *Hibiscus rosa-sinensis* L.
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PP-52 The bioactivities of total extract and fractions from *Codonopsis javanica* (blume) root
Hai Long Tran, Ton Duc Thang University, Vietnam

Organic & Medicinal Chemistry

<PP-01>

A machine-learning model to predict P-gp inhibitors

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Keywords: Multidrug resistance, scoring function, machine-learning, P-glycoprotein

Background: Various therapeutic methods have been developed to combat cancer, with chemotherapy playing a prominent role. However, multidrug resistance has proven to be a major hurdle. This phenomenon is primarily associated with efflux pumps, one of which is P-glycoprotein (P-gp). Currently, there is no available drug that inhibits this protein in clinical settings. The application of computer-aided drug design, or more specifically, of artificial intelligence and modern computer techniques has become a prevailing trend, set to dominate the future. This project aims to construct a new classification model for structure-based virtual screening of P-gp inhibitors using random forest, a supervised learning algorithm.
Methods: Experimental data from ChEMBL and Protein Data Bank (a 3D P-gp structure and molecules *in vitro* tested as its inhibitors) were retrieved and processed using our in-house protocol. An unbiasing method, Asymmetric Validation Embedding (AVE), was used to split these molecules into a training set and a test set. Molecular docking was carried out with Smina, after which all docked complexes were encoded as protein-ligand extended connectivity (PLEC) fingerprints. These PLEC features were then employed as input for training and testing a random forest binary classifier, using the *RandomForestClassifier* function from the *sklearn* Python package. The screening performance on the test set of this model was evaluated and compared with that of Smina's native classical scoring function.
Results: The data set retrieved from ChEMBL was unbiased, with a negligible AVE bias value (0.004) after 14 iterations. It consists of 1106 molecules in total, with an active-to-inactive ratio of 1/4.073 and a training-to-test ratio of 80/20. Our random forest-based machine-learning scoring function (RF-based MLSF) gave superior performance (EF3% = 3.33) compared to Smina's classical SF (EF3% = 1.67). Further analyses revealed that the results of our RF-based MLSF aligned well with experimental findings, with the most potent hit retrieved among the top 3%-ranked molecules having an IC50 of 50 nM. Furthermore, true hits predicted by this RF model and Smina's SF exhibited diverse chemical structures.
Conclusions: This study successfully constructed a data set with minimal bias, suitable for training and testing new ML models. Moreover, we successfully developed and validated a P-gp-specific binary classification model for predicting its inhibitors, using the random forest algorithm. The model showcased better performance than Smina's classical SF in terms of early true hit enrichment and selected true hits having low IC50s *in vitro*.

<PP-02>

Discovery of natural interleukin 36γ small molecule inhibitors by pharmacophore screening, docking analysis, ADMET prediction, and molecular dynamics simulations

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Keywords: 3D-Pharmacophore, AMET, docking, interleukin 36γ, molecular dynamics

Background: Interleukin-36 gamma (IL-36γ) is a member of the interleukin-1 cytokine family. It is involved in immune cell activation, antigen presentation, and pro-inflammatory factor production. The important target cells of IL-36γ are the keratinocytes. Many recent studies have found a relationship between IL-36γ dysregulation and disease activity in inflammatory autoimmune diseases, such as psoriasis, systemic lupus erythematosus, and rheumatoid arthritis. Therefore, inhibitors of IL-36γ are the potential target in the treatment of these inflammatory autoimmune diseases. A-552 was identified as the most potent antagonist of human IL-36γ by Viktor Todorović et all. The interaction between A-552 and IL-36γ is the basis for this study.

Methods: A total of 57,424 natural compounds from the Traditional Chinese Medicine library were screened. The 3D-pharmacophore model was built using MOE 2019.0102 software based on the interaction of interleukin 36 and A-552. Compounds satisfying the 3D-Pharmacophore model were minimized energy by the software Open Babel 2.4.0. The FlexX tool in LeadIT 2.1.8 software provided by BioSolveIT GmbH was used to perform molecular docking. Compounds with a docking score lower than A-552 (-36.7063 kJ/mol) were evaluated for ADMET by the pkCSM server. Finally, the substances were simulated for molecular dynamics using Gromacs 2022.4 software, and the binding free energies were calculated using the molecular mechanics generalized Born surface area (MM/GBSA) method to identify potential compounds that inhibit interleukin 36γ activity.

Results: Initially, 57,424 small molecules were screened based on the pharmacophore model. Then, 2,891 compounds were selected for further evaluation based on the molecular docking scores. After ADMET studies, molecules TCM184 (-49.2168 kJ/mol), TCM6727 (-40.9385 kJ/mol), TCM2246 (-37.7439 kJ/mol), and TCM729 (-37.531 kJ/mol) were selected for further verification. By molecular dynamics analysis, molecule TCM184 maintains a stable conformation with the target protein and has a lower free binding energy than A-552, so it has the chance to become an inhibitor of interleukin 36γ.

Conclusions: Through structure-based pharmacophore modeling, virtual screening, molecular docking, ADMET approaches, and molecular dynamics simulation, the natural compound TCM184 can be used as a small molecule inhibitor of IL-36γ.

<PP-03>

Synthesis, physiochemical characterization, and bioactivity of α-mangostin integrated cellulose hydrogel

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Keywords: *α*-mangostin, cellulose hydrogel, nano polydopamine, antioxidant activity

Background: Hydrogel is a 3D network composed of multiple polymer chains crosslinked to form structures with unique properties. Integration of functional polymers such as polydopamine (PDA) or *poly(β-amino ester)* (PBAE) into hydrogel structure brings forth fascinating characteristics such as drug loading capacity, drug release capacity or pH sensitivity. Alternatively, *α*-mangostin can be integrated with hydrogels to create an extended-release system, improving the bioavailability of this compound.
Methods: Cellulose solution were physically crosslinked in NaOH/urea medium with functional polymers (PDA or PBAE), and *α*-mangostin to form cellulose hydrogel beads. Alginate hydrogel beads were prepared by divalent chemical crosslinking sodium alginate solution in calcium chloride medium with functional polymers (PDA). Physiochemical properties of hydrogels were studied using various techniques including FT-IR, ^{13}C CP-MAS NMR, TGA-DSC, and SEM. Antibacterial capabilities of *α*-mangostin integrated hydrogels were explored by detecting changes regarding minimum inhibitory concentration against *S. Aureus* and antioxidant activity of hydrogels were analysed using ABTS free radical scavenging method. *In vitro* drug release tests were performed in various pH.
Results: FT-IR, ^{13}C CP-MAS NMR results indicating cellulose structure did not change chemically during and after hydrogel formation. TGA-DSC revealing decomposition temperature at 340 – 427 ^{o}C. Observation obtained by SEM showing high porous density appropriate for drug loading applications. The cumulative drug release at pH 8.4 medium reaching higher than that at pH 7.4 and pH 1.2 medium, indicative of pH sensitivity for controlled delivery. The addition of functional polymers (PDA or PBAE) into hydrogel structures gave rise to faster and more intense liberation of *α*-mangostin in pH 8.4 medium. Drug release kinetic of hydrogels providing further insights into changes in polymeric networks following liberation of drug content. Hydrogel integrated with *α*-mangostin exhibit antibacterial properties at MIC of 80 mg mL^{-1}. The addition of PDA into hydrogel structures along with *α*-mangostin brings forth antioxidant capabilities at IC_{50} of 50 mg mL^{-1}.
Conclusion: These results imply the possible application of *α*-mangostin integrated PDA or PBAE cellulose hydrogel as a potential pH-controlled drug delivery system with antibacterial and antioxidant properties.

<PP-04>

Synthesis and characterization of isosorbide-based biodegradable poly(*β*-amino ester) for drug delivery applications

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Keywords: Poly(*β*-amino ester), nanoparticle, isosorbide, drug delivery, biodegradable

Background:
Poly(β-amino ester) (PBAE) is a polymer that is synthesized by the Michael addition reaction between an acrylate and an amine. This versatile material shows great promise in a wide range of applications, including gene delivery, anticancer drugs, and antimicrobial agents. Isosorbide, which is derived from sorbitol and bears a structural similarity to glucose, offers an excellent opportunity to harness its bioresources for the development of a novel therapeutic delivery material. In this study, we propose the incorporation of isosorbide into PBAE, aiming to create an innovative material with enhanced therapeutic capabilities.
Methods: The isosorbide diacrylate monomer was synthesized through the esterification of isosorbide with acryloyl chloride. The resulting monomer was then reacted with piperazine to form PBAE incorporating isosorbide. The chemical structure of the obtained products was confirmed using various spectroscopic techniques, including FT-IR, ^{1}H NMR, ^{13}C NMR, and UV-Vis spectroscopies. To assess the potential of these polymers in enhancing the biological activity of drugs, they were loaded with tartrazine, levofloxacin, ciprofloxacin, and α-mangostin. The formation of nanoparticles and their size distribution were determined using dynamic light scattering technique. Furthermore, the inherent antimicrobial activity of the loaded antibiotics and α-mangostin was evaluated by measuring the change in minimum inhibitory concentration against *S. aureus*, *P. aeruginosa*, *E. coli*, and *B. subtilis*. The antioxidant activity of the nanocomplex particles was investigated using the ABTS free radical scavenging method.
Results: The spectrum analysis results successfully confirm the chemical structure of the synthesized polymer. Both PBAEs have demonstrated the ability to form nanoparticles with the drugs, exhibiting sizes ranging from 80 to 200 nm. Furthermore, the antimicrobial activity of the antibiotics showed significant improvement when combined with PBAE. Additionally, PBAE was found to enhance the antioxidant activity of α-mangostin. The IC_{50} value of mangostin decreased from 8.07 μg mL^{-1} to 6.02 μg mL^{-1} when incorporated into PBAE, suggesting an improved antioxidant potential.
Conclusions: These findings indicate that the inherent biological properties of PBAE make it a promising candidate for polymer-based nanocarriers in drug delivery systems.

<PP-05>

Synthesis and surfactant-mediated modification of nanocrystalline cellulose for *α*-mangostin delivery

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Keywords: cellulose, *α*-magostin, surfactant-mediated nanocellulose, antioxidant

Background: Nanocrystalline cellulose (NCC), a natural polymer obtained from abundant native cellulose, showcases remarkable physical, chemical, and biological characteristics. It exhibits exceptional attributes like superior mechanical strength, stiffness, lightweight nature, biocompatibility, and renewability. These advantageous properties make it highly suitable for the development of advanced drug delivery systems, whether employed as an additive or a carrier.

Methods: Microcrystalline cellulose derived from cotton fiber underwent hydrolysis using hydrochloric acid to serve as the starting material for nanocellulose synthesis. NCC were prepared through a method involving sulfuric acid hydrolysis, accompanied by ultrasonication and homogenization. The resulting nanocelluloses were further modified using different surfactants, namely cetyltrimethylammonium bromide (CTAB), sodium decyl sulfate, tween 80, or decyl glucoside. This surfactant-mediated nanocelluloses were then explored for their potential as a sustained release drug delivery system of α-mangostin. The chemical structure and morphology of the resulting nanocellulose materials were analyzed using techniques such as FT-IR, TGA-DSC, DLS, SEM, and TEM. The antioxidant activity was evaluated using the ABTS assay, while the antibacterial activity was determined by employing the broth microdilution method to ascertain the minimum inhibitory concentration (MIC) against *S. aureus*.

Results: Nanocellulose with an average particle size of approximately 190 nm was successfully synthesized from cotton fiber. The surfactant-mediated modification of nanocellulose resulted in a significant improvement in α-mangostin binding capacity, reaching up to 292.21 ± 2.20 mg g^{-1}. Among the surfactants tested, the cationic surfactant CTAB proved to be highly efficient as a binding agent for α-mangostin. This modified nanocellulose exhibited the highest antioxidant activity, with an IC_{50} value of 3.91 ± 0.35 µg mL^{-1}, and demonstrated potent antibacterial activity, with a MIC of 0.2 µg mL^{-1}.

Conclusions: The results underscore the potential of utilizing surfactant-mediated nanocellulose in the development of drug delivery systems and highlighting its versatility for a wide range of pharmaceutical applications.

<PP-06>

Chemical constituents and antioxidant evaluation of *Ochna integerrima* (Lour.) Merr. stem

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Keywords: Antioxidant activity, chemical constituents, flavonoids, *Ochna integerrima*

Background: *Ochna integerrima* - "Mai vang" is a medicinal plant belonging to the *Ochnaceae* family. This species has been reported to possess various pharmacological activities, including antioxidant, anti-inflammatory. Traditionally, the stems have been used as a digestive tonic, antidysentery, and antipyretic. However, its chemical components and the antioxidant activity of extracts are still not fully demonstrated.
Methods: We displayed the antioxidant potential of extracts (*n*-hexane, dichloromethane, EtOAc, *n*-butanol, aqueous, and MeOH extracts) from the stem using a DPPH assay. Moreover, the total phenolic and flavonoid contents (TPC and TFC) were determined using Folin-Ciocalteu and $AlCl_3$ colorimetric assays. Thereafter, the chemical components from the active extract were investigated. The structures of the isolated compounds were determined by HRESIMS, 1D NMR spectra, and comparison with published data.
Results: All the extracts, except for the *n*-hexane showed significant antioxidant activity with IC_{50} values ranging from 9.57 ± 0.21 to 45.32 ± 0.21 µg/mL. Moreover, the TPC and TFC values were well-correlated with DPPH capacity. The five isolates, 6*β*,17-dihydroxy-*ent*-kauran-19-oic acid (**1**), syringaresinol (**2**), calodenone (**3**), pinocembrin (**4**), and daucosterol (**5**) were isolated from dichloromethane extract of *O.integerrima* stems. Compounds **1** and **2** were isolated for the first time from this species.
Conclusions: The five isolated compounds **1**-**5** were isolated from dichloromethane extract of *O. Integerrima* stems. This species may be a good candidate for antioxidant activity. Therefore, further phytochemical investigations and the antioxidant activities of secondary metabolites are required to elucidate the pharmacological properties.

<PP-07>

Polycation-modified Fe(III)-MOF loaded with methotrexate and Pt(IV) prodrug for synergistic anticancer therapy

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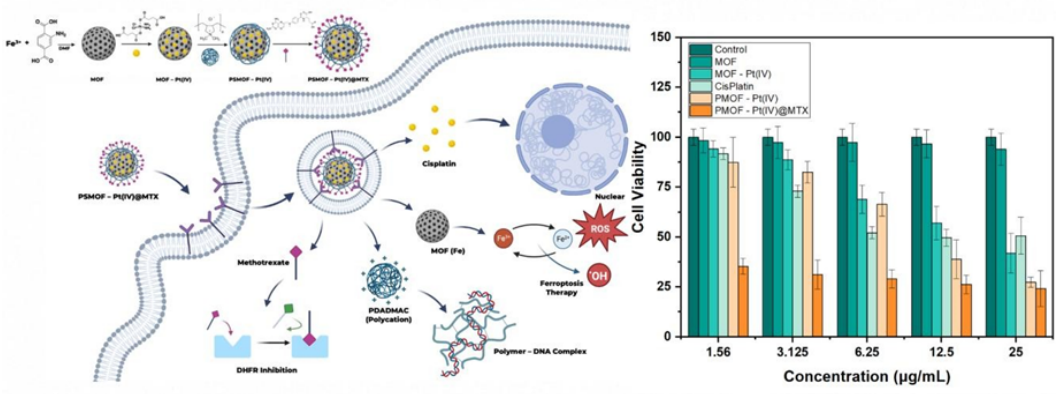
Keywords: metal−organic frameworks, Pt(IV) prodrug, polycation, Methotrexate, synergistic anticancer therapy

Background: Chemotherapy is the most common intervention in treating cancer, yet severe adverse drug reactions following therapy result in prolonged hospitalization. Thus, the development of medicines with chemo-synergistic actions is urgent. As a drug nanocarrier, Fe-based metal- organic frameworks (MOFs), specifically MIL-101(Fe)-NH_2 can release both Fe(III) ions and drug, such as Cisplatin, intracellularly to afford Ferroptosis and chemotherapy, respectively. Meanwhile, as the outside surface of this nanocarrier exhibits negative charges, polycationic PDADMAC is coated on the surface to link the nanocarrier with Methotrexate (MTX), an antimetabolite that also serves as a ligand for receptor-mediated endocytosis to breast cancer cells.

Methods: MIL-101(Fe)-NH_2 (Fe(III)-MOF) was synthesized under solvothermal conditions, and the Pt(IV) prodrug was attached to the MOF via amide bond formation to afford MOF-Pt(IV). The MOF-Pt(IV) was then coated with polycation PDADMAC, resulting in PMOF-Pt(IV). Finally, PMOF-Pt(IV)@MTX was obtained by loading MTX into PMOF-Pt(IV). The nanomedicine was characterized by PXRD, SEM-EDS, zeta potential, ICP-AES, and its cytotoxic efficacy was tested on 4T1 breast cancer cells via MTT assay.

Results: The zeta potential value (ζ) of PMOF-Pt(IV)@MTX is +26.48 mV which is lower than that of PMOF-Pt(IV). The decrease in value is an expected outcome and proves the successful loading of MTX on the surface of PMOF-Pt(IV). Meanwhile, the ζ value of MOF and MOF- Pt(IV) is negative, confirming that PDADMAC successfully modified the surface of MOF- Pt(IV). Concurrently, PMOF-Pt(IV)@MTX has a high MTX and Pt(IV) prodrug loading capacity of 26 and 25 wt%, respectively. Importantly, the cytotoxicity of PMOF-Pt(IV)@MTX is potent even at low doses. The cell viability of 4T1 human breast cancer cells decreased after exposure to PMOF-Pt(IV)@MTX for 24 h. At 25 μg/mL, PMOF-Pt(IV)@MTX exhibited 76% cytotoxicity, higher when compared to other materials. The calculated IC_{50} is 0.11 μg/mL, which is remarkably lower than that of other materials, suggesting the superior therapeutic effect of this nanomedicine.

Conclusions: The successfully synthesized PMOF-Pt(IV)@MTX showed the promising capability to kill breast cancer cells. The current properties of PMOF-Pt(IV)@MTX are good indications of a highly selective nanomedicine with synergistic actions against breast cancer.



<PP-08>

Transmembrane amyloid β-peptide structures: *In silico* study

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Amyloid beta (Aβ) peptides are considered the major causative agents of Alzheimer's disease (AD). In a widely accepted mechanism for AD pathogenesis, Aβ peptides are proposed to play multiple roles in damaging brain cells and their synaptic communications. Due to the heterogeneous nature Aβ oligomers, their in vivo structures have not been understood. Most experimental and computational studies favored β-rich structures of Aβ as observed in Aβ fibrils. To determine the putative structures of the transmembrane Aβ oligomers, the temperature replica exchange molecular dynamics (REMD) simulations with an explicit solvent has been employed to monitor its structural change when the membrane DPPC lipid bilayers is induced. The initial structure of the oligomers was modelled based on the current low-resolution data of these conformations. The physical insights into the forming transmembrane Aβ oligomers probably enhance the AD therapy.

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Pharmacology & Clinical Pharmacy

<PP-09>

Anti-cancer effects of indirubin derivative against acute myeloid leukemia

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Keywords: AML, FLT3/RET dual-target inhibitor, Indirubin derivative, PLM-101

Background: Acute myeloid leukemia (AML) is a prevalent form of leukemia in adults. As its survival rate is low, there is an urgent need for new therapeutic options. In AML, *FMS-like tyrosine kinase 3* (*FLT3*) mutations are common and have negative outcomes. However, current FLT3-targeting agents, Midostaurin and Gilteritinib, face two significant issues, specifically the emergence of acquired resistance and drug-related adverse events leading to treatment failure. *Rearranged during transfection* (*RET*), meanwhile, is a proto-oncogene linked to various types of cancer, but its role in AML has been limited. A previous study showed that activation of RET kinase enhances FLT3 protein stability, leading to the promotion of AML cell proliferation. However, no drugs are currently available that target both FLT3 and RET.
Methods: Human AML cell lines MV4-11, MOLM-13, and MOLM-14 were used. AML cell viability was analyzed by WST-8 assays. Apoptosis and cell cycle analyses were performed by flow cytometry. Activities of downstream signaling pathways of FLT3 were estimated by immunoblottings using phospho-specific antibodies. Flank and orthotopic xenograft mouse models were used to assess in vivo anti-cancer effects of PLM-101.
Results: In this study, we propose PLM-101, a synthetic derivative of indirubin from the traditional Chinese medicine (TCM) *indigo naturalis*, as a promising anti-leukemic therapeutic option. Its pharmacological mechanism is the inhibition of FLT3 and its downstream signaling pathways, including the phosphoinositide 3-kinase (PI3K)/AKT and Ras/extracellular signal-regulated kinase (ERK) pathways. Additionally, PLM-101 induces autophagic degradation of FLT3 by targeting RET, thus providing an additional mechanism to the stronger anti-leukemic activity of FLT3/RET dual-targeting inhibitors relative to that of FLT3 single-targeting inhibitors.
Conclusions: This study presents a novel FLT3/RET dual-targeting inhibitor, PLM-101, that exhibits potent anti-leukemic activity *in vitro* and *in vivo*. PLM-101, therefore, should be considered as a potential therapeutic option for AML harboring both *RET* and *FLT3* mutations.

<PP-10>

Evaluate the efficacy of early use of remdesivir among patients with COVID-19

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Keywords: COVID-19, Remdesivir, efficacy

Background: Currently, the use of Remdesivir for COVID-19 patients has become popular. However, evidence regard to the efficacy of early use of remdesivir remains limited. The study aims to evaluate the efficacy of early use of Remdesivir among patients with COVID-19.
Methods: A retrospective cross-sectional study was conducted at Cu Chi COVID-19 Treatment Hospital from June 2020 to February 2022. Data were collected from 359 medical records of COVID-19 patients who used Remdesivir. Logistic regression analyses were used to examine the relation between demographic characteristics and clinical features, and mortality in COVID-19 patients. Linear regression analysis was performed to assess how the day of using Remdesivir use impacted the time to recovery among COVID-19 patients. A P-value less than 0.05 was considered to be statistically significant.
Results: Among 359 patients in the study population, 66.0% were female, and 35.6% were under 60 years old. 70.8% of patients recovered based on the study's clinical improvement assessment. Patients who died within 14 days accounted for 10.9%. The average time for patients to recover and hospital stays were 9.56 ± 6.19 days and 13.14 ± 6.36 days, respectively. Regarding logistic regression analyses, factors of COVID-19 patients that were associated with mortality included age over 60 years (OR = 5.02; 95% CI = 1.69 – 14.96), pre-hospital status: no hospitalization, limited activities and/or need for home oxygen (OR = 5.73; 95% CI = 2.03 – 16.17), patient condition at pre-hospitalization: on non-invasive ventilation (via mask) or high-flow oxygen (HFNC) (OR = 6.80; 95% CI = 1.57 – 29.36), day of using Remdesivir: from the third day after being diagnosed with COVID-19 (OR = 3.39; 95% CI = 1.17 – 9.82). According to linear regression analysis, when the day of using Remdesivir increased one day, the average time to recovery increased by 0.59 days (95% CI = 0.26 – 0.92).
Conclusions: Early use of Remdesivir among patients with COVID-19 can improve recovery and reduce time to recovery, length of hospital stays, and mortality risk. Therefore, it is crucial to implement the early use of Remdesivir in the treatment of patients COVID-19 for better efficacy.

<PP-11>

Intervention of pill card to improve medication adherence among HIV patients at one primary health care in Bandung Indonesia

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Keywords: Adherence to medication, HIV Patients, Pillcard

Background: Medication adherence is very important for HIV patients. Poor adherence to antiretroviral therapy is associated with less effective viral suppression, which risks immediate health as well as creates permanent treatment resistance to that particular agent or group of agents within a given combination therapy regimen. Medication reminder card or Pill Card is one of the intervention tools to improve patient medication adherence. This study aims to determine the effect of Pill card intervention on medication adherence in HIV patients.

Methods: The pre-experimental type one-group pretest–posttest design was conducted in purposive samples of HIV patients period from February to April 2023 at one primary health care in Bandung Indonesia. Pill card intervention was given for 1 month. Data on medication adherence was obtained from a standard Medication Report Adherence Scale (MARS-5) questionnaire and Pill count. Univariate analysis was used to describe the distribution of each dependent variable while bivariate analysis was performed to determine the correlation between the two paired variable data, before and after being given the Pill card intervention and the effectiveness of the Pill card intervention.

Results: Of the 93 participants, the demographic showed mostly were male (92.47%, n=86), aged range 26-35 years old (45.16%, n=42), as an employee (82.79%, n=77), high school level (59.13%, n=55), and less than 1 year of treatment duration (41.93%, n=39). Based on the MARS questionnaire before the intervention, 56.76% of the participants (50/93) were categorized with high adherence and 46.24% (n=43) with low adherence whether adherence level was higher (52.69%, n=49) than non-adherence level (47.31%, n=90) using pill count method. After the intervention, high adherence level was higher (83.87%, n=78) and low adherence level was lower (16.13%, n=15) using MARS questionnaire. The pill count method resulted in adherence level of patients was higher (75.27%, n=70) and non-adherence level was lower (24.73%, n=23) with p-value of $p<0.000$ and $p=0.001$ respectively.

Conclusions: Pill card intervention was shown to significantly improve patient medication adherence both based on assessment using the MARS-5 questionnaire and the pill count method.

<PP-12>

Blood pressure lowering effect of Jamaica cherry (*Muntingia calabura* L.) leaves and its fraction

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Keywords: blood pressure, antihypertensive, epinephrine, fraction, *Muntingia calabura* L.

Background: Hypertension is a chronic disease defined as an increase in systolic blood pressure >140 mmHg and diastolic blood pressure >90 mmHg, with increasing prevalence. The use of herbal medicines is increasing, especially for treating and managing chronic diseases such as hypertension. Muntingia calabura L. (Jamaica cherry) is one of the medicinal plants that empirically has been used to lower blood pressure. Jamaica cherry is known to cause vasodilation in N(gamma)-nitro-L-arginine methyl ester-induced hypertensive animal models. However, there are no studies on adrenergic receptor activity. This study aims to determine the antihypertensive activity of ethanol extract, the fractions of Jamaica cherry leaves in the epinephrine-induced hypertensive animal model, and the compounds contained in the active fraction.
Methods: In examining the antihypertensive effect, test doses of Jamaica cherry leaves extract were 50, 100, and 200 mg/kg BW. The test dose of water, n-hexane, and ethyl acetate fraction was 100 mg/kg BW. Blood pressure was measured using a non-invasive CODA® tail-cuff blood pressure system. Thin layer chromatography (TLC) was performed to observe the compounds in the extract/fraction.
Results: Epinephrine-induced hypertensive animal model is an approach to studying adrenergic receptor activity. Epinephrine activates β-1 and β-2 receptors, increasing heart rate and contractility and dilation of muscle arterioles. The results of the antihypertensive activity test showed that the ethanol extract of Jamaica cherry leaves at a dose of 100 mg/kg BW had the best inhibitory effect of increased systolic and diastolic blood pressure, respectively, 39,04 and 49,37%. Ethyl acetate fraction showed the best inhibitory effect of increased systolic and diastolic blood pressure, 59.48 and 74.70%.
Conclusions: Extract and fractions of Jamaica cherry leaves can reduce blood pressure in epinephrine-induced hypertensive rats. Ethanol extract and active fraction as antihypertensives contain quercetin and kaempferol.

<PP-13>

Inappropriate prescribing of antipsychotic drugs in elderly patients at a psychiatry hospital in Viet Nam using stop/start criteria and APID index

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Keywords: psychotropic medications, inappropriate prescribing, STOPP/START criteria, APID index.

Elderly patients are at a higher risk of experiencing serious adverse drug reactions due to the use of psychotropic medications. Potentially inappropriate prescribing (PIP) is a frequent cause of drug-related side effects in this population. Ensuring the safety and effectiveness of drug treatment with antipsychotic agents in elderly patients requires the control and prevention of PIP.

This study aimed to determine the rate of PIP in inpatient prescriptions at a Psychiatry Hospital using the STOPP/START criteria and APID criteria, as well as to evaluate factors associated with PIP occurrence.

A descriptive cross-sectional study was conducted using medical records of patients who had been prescribed at least one psychotropic drug and were hospitalized at Bien Hoa Central Psychiatry 2 Hospital in Dong Nai province between January 2017 and April 2021. The rationality of drug use was assessed based on the STOPP/START criteria for potentially inappropriate prescribing in older people (version 2, 2014) and the APID criteria.

A total of 411 medical records were included in the study. According to the STOPP/START criteria, 74 records (18%) met at least one STOPP criterion in the prescription of central nervous system and psychotropic drugs, resulting in a total of 91 potentially inappropriate medications (PIMs) and no potentially prescribing omissions (PPOs). Among these, 27.4% of prescriptions lacked evidence-based clinical indications. Phenothiazines were the most commonly inappropriately prescribed drugs as first-line treatment, despite the availability of safer and more effective alternatives (23.9%). The number of drugs per prescription was associated with the risk of inappropriate prescribing (odds ratio = 1.30, 95% confidence interval 1.13-1.50). No statistically significant associations were found for patient characteristics (gender, age, Charlson comorbidity index) or physician characteristics (age, gender, and qualification).

Using the APID index, the mean APID sum score for all 411 records was 8.15 ± 6.12, ranging from 0 to 31. Approximately 79.8% of the records had at least one PIP. There were statistically significant associations between the number of medications prescribed and the risk of PIP.

In conclusion, this study highlights the need for improvement in the prescribing practices of antipsychotic drugs for elderly patients. Furthermore, patients prescribed a higher number of medications were more susceptible to the risk of PIP. Interventions should be implemented to reduce inappropriate prescriptions in the elderly, such as restricting unnecessary drug use and considering the safety and efficacy of first-line treatment drugs.

<PP-14>

Depression status among type 2 diabetes patients in Gia Dinh people's hospital

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Keywords: depression, diabetes mellitus type 2, Patient Health Questionnaire

Background: Depression is increasing among patients with type 2 diabetes in Vietnam. The relationship between depression and diabetes has a negative effect on the patient's health status. The objectives of this study were to investigate the status of depression in patients with type 2 diabetes and the correlation between these two diseases.

Methods: A descriptive cross-sectional study at the Endocrine Department of Gia Dinh People's Hospital from March to June 2022. The study included 270 adult type 2 diabetes patients. Data were collected on demographic characteristics, health behaviors, and clinical characteristics. Depression was evaluated by the Patient Health Questionnaire – 9 (PHQ-9). Logistic regression analyses were used to examine which factors were associated with depression among type 2 diabetes patients. Linear regression analyses were performed to determine the impact of depression on type 2 diabetes disease. A P-value less than 0.05 was considered to be statistically significant.

Results: Among 270 patients with type 2 diabetes in the study population, 42.6% were diagnosed with depression according to the PHQ-9 scale. The proportions for mild, moderate, relatively severe, and severe depression were 33.0 %, 8.5 %, 0.7 %, and 0.4 %, respectively. In multivariable logistic regression analyses, only gender was associated with depression (OR = 2.054, 95 % CI = 1.159-3.641). Regarding linear regression models, when PHQ-9 score increased by 1 point, HbA1c increased by an average of 0.059 % (® = 0.059, 95 % CI = 0.001-0.117), fasting plasma glucose increased by an average of 0.15 mmol/l (® = 0.15, 95 % CI= 0.061-0.239) and the number of complications of type 2 diabetes increased by an average of 0.04 (® = 0.04, 95 % CI = 0.010-0.070).

Conclusions: The rate of depression was high in patients with type 2 diabetes at Gia Dinh People's Hospital. Additionally, depression can reduce the ability to control blood glucose, HbA1c, and complications in patients with type 2 diabetes. Therefore, it is necessary to screen for depression in patients with type 2 diabetes to improve treatment efficiency and quality of life for patients.

Pharmaceutics & Industrial Pharmacy

<PP-15>

Preparation of cough lozenges from the Vietnamese traditional remedy “Bach Bo Bo Phe”

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Keywords: Cough relief, compressed tablets, Bach bo bo phe, modern formulation, traditional medicine

Background: Recently, the use of traditional medicine is significantly increased because of its treatment effficacy and minimized side effects. “Bach bo bo phe” is a popular cough-relieving remedy, comprising different medicinal herbs, such as: *Stemona tuberosa, Ophiopogon japonicus, Glycyrrhiza uralensis, Platycodon grandiflorus, Pouzolzia zeylanica* and *Fructus Terminaliae chebulae*. Nevertheless, there are associated issues in the current commercialized products including the large use volume, unpleasant palatability and intolerance for diabetic patients. Formulating compressed tablets is expected to resolve these problems for drug administration purposes.
Methods: The quality of the input medicinal herbs and extracts were controlled according to the standards in the Vietnam Pharmacopoeia V. The formulation of compressed tablets was developed, optimized and characterized according to the established in-house standards. The palability of the obtained tablets was assessed on 30 volunteers. Finally, its *in vitro* antibacterial activity was proved on *MSSA strain.*
Results: All input materials met the quality standards in the Vietnam Pharmacopoeia V. The compressed tablets were successfully optimized and complied with the in-house standards, possessing a taste and odor appraised by all involved volunteers. Especially, the optimized tablet was showed to have an antibacterial effect on *MSSA*.
Conclusion: This study successfully developed the traditional remedy "Bach Bo Bo Phe" into a tablet form complying with medical standards for mass consumption.

<PP-16>

Formulation of mouthwash solution containing microemulsion of *Ocimum gratissimum* essential oil for antibacterial action in the oral cavity

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Keywords: Microemulsion, essential oil, *Ocimum gratissimum*, mouthwash, antibacterial

Background: White basil (*Ocimum gratissimum*) is a potent essential oil to prevent the overgrowth of the oral bacterial flora. Nevertheless, its poor water solubility and high volatility limit its real-life application. This study focused on the development of a novel formulation to increase the solubility and stability of this potent essential oil.
Methods: Microemulsion was chosen and formulated with distilled water, essential oil as the oil phase and surfactants. The ratio of each component was investigated and optimized using ternary diagram. The selection criteria included the formulation with the highest water proportion and smallest surfactant one. The optimized microemulsion was characterized in terms of size, and phase stability at harsh conditions. Eventually, a formulation of mouthwash was developed, quality controlled and evaluated for its palatability on 30 randomly selected volunteers.
Results: The optimized microemulsion comprised essential oils (1%), distilled water (55%), tween 80 as co-surfactant (7%), isopropanol (7%), and labrasol as surfactant (30%), with a high stability after a month under accelerated conditions. In addition, the obtained nano-formulation met the evaluation criteria and possessed an effective antibacterial effect within 30 seconds of exposure to *Streptococcus mutants*. Finally, a mouthwash containing essential oil (1%), optimized in terms of palatability with menthol (0.5%), aspartame (0 .5%), and mannitol (1.5%) was successfully prepared and received positive responses from all involved volunteers.
Conclusion: This study successfully developed a microemulsion containing white basil essential oil and its mouthwash preparation, complying with quality and stability standards for commercial purposes.

<PP-17>

Zwitterionic cyclodextrin nanocarrier for tumor targeted drug delivery

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Keywords: tumor-targeting, nanocarrier, drug delivery

Background: Renal-clearable nanocarriers have a high potential in cancer-targeted drug delivery. However, reports on the optimal design of nanocarriers to improve drug retention in tumors while minimizing off-target tissues distribution are limited. Herein, we present a tailored structure of a renal-clearable zwitterionic β-CD derivative (PBA-(ZW)-CD) for colorectal cancer (CRC)-selective anticancer drug delivery.
Methods: Various CD derivatives with different charged moieties and spacers were synthesized and screened for colloidal stability. CD derivatives were complexed with a fluorescence dye (ACy7) and their biodistribution profiles were evaluated using near-infrared imaging. CRC targetability, organ distribution, and renal clearance of CD derivatives were screened in the form of ACy7 inclusion complexes. From these screening results, PBA-(ZW)-CD was selected as the optimized structure, with enhanced tumor selectivity and reduced off-target accumulation. Doxorubicin and ulixertinib were separately loaded into PBA-(ZW)-CD to evaluate the feasibility as a CRC-selective drug delivery system. The PBA-(ZW)-CD/drug inclusion complexes were applied in combination therapy for CRC, and the therapeutic efficacy and safety was investigated.
Results: PBA-(ZW)-CD exhibited a high tumor-to-background ratio of 3.7–4.1. Inclusion complexes of doxorubicin and ulixertinib with PBA-(ZW)-CD enhanced tumor accumulation of doxorubicin and ulixertinib. Their facilitated elimination and tumor penetration were verified through mass-spectrometric quantitation and imaging. The improved antitumor efficacy of PBA-(ZW)-CD/drug combination therapy was demonstrated in heterotopic and orthotopic CRC models, with tumor size reduction by 52.0% and 76.2%, respectively, compared to free drug combination.
Conclusions: The optimized complex formulation showed improved tumor retention and facilitated elimination from normal tissues. These results suggest that PBA-(ZW)-CD can offer a promising nanoplatform for CRC-targeted anticancer drug delivery.

<PP-18>

Development of nanoformulation containing fluconazole and ibuprofen to tackle the *Candidiasis*'s fluconazole-resistance phenomenon

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Keywords: Candidiasis, fluconazole-resistance, ibuprofen, nanoformulation

Background: The emergence of the drug-resistance phenomenon in fungal infections, particularly fluconazole in candidiasis, poses a real threat to the public health. Several studies have demonstrated the potential of the synergistic effect of fluconazole and ibuprofen to address this issue. However, the poor solubility of ibuprofen as well as a formulation containing these two active ingredients remain a gap for the use of this combination in reality. This research aims to construct a nano-formulation to co-deliver these active ingredients and an *in-situ* gel to facilitate the use of these drugs in oral candidiasis.
Methods: Micellar nano-formuation using appropriate solvents and surfactants was developed and optimized. The nanoplatform was characterized in terms of its visual appearance, pH, particle size, and stability. The gel-forming excipient, poloxamer 407, was studied at various concentrations to form the *in-situ* gel. The obtained gel was assessed for visual appearance, pH, stability, spreadability and palatability on 30 randomly selected volunteers. The synergistic activity and the benefit of nano-formuation in antifungal properties were *in vitro* assessed against both fluconazole -sensitive and -resistant strains.
Results: The optimized nano-formulation consists of fluconazole 0.5%, ibuprofen 0.125%, tween 80 2.5%, ethanol 2.5%, and water 94.38%, with a nano-size of 11.7±0.2 nm. Poloxamer 407 at a concentration of 15% exhibited optimal gel formation for *in-situ* application, meeting predetermined quality assessment criteria. The final gel product received positive feedbacks from all involved volunteers. *In vitro* antifungal tests confirmed a significant synergistic effect of fluconazole and ibuprofen on the resistant strain, without any observable effects on the sensitive one.
Conclusions: This study successfully developed a nanosized system and an *in-situ* gel formulation containing fluconazole and ibuprofen with a high potential to solve the problem of fluconazole-resistance phenomenon.

<PP-19>

The application of ion-exchanging resin in fexofenadine orally disintegratting tablet formulation

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Keywords: Fexofenadine hydrochloride, Taste masking, Ion exchange resin, Orally disintegratting tablet, Amberlite IRP88

Background: Fexofenadine hydrochloride is a selective, non-sedating H1 receptor antagonist which are widely prescribed for seasonal allergic rhinitis and chronic idiopathic urticaria especially for children. This medicinal drug has a highly unpleasant bitter taste – the reason why this compound prepared as coating tablets. Even so, there are groups of special patients who have problem in swallowing the whole tablet. This study aims to prepare a formulation of fexofenadine hydrochloride 30 mg orally disintegratting tablet which has taste-masked, short disintegrating time and high dissolution rate.
Methods: Fexofenadine hydrochloride was taste-masked by making a drug – ion exchange resin complex. The orally disintegratting tablet was prepared by direct compression method, using taste-masked complex and superdisintegrants excipients.
Results: The drug-resin complex was masked the bitter taste successfully, drug loading capacity reached 92% at the dug:resin ratio 1:1. The orally disintegratting tablet had a short disintegrating time, wich was prepared from drug-resin complex and 6% (w/w) of superdisintegrants, without any unpleasant bitter taste. The dissolution rate of the tablet reached 85% release before 30 minutes. The ion exchange resin improves flowability and compressibility of powdered excipients, make it possible to application direct compression method during tablet's production.
Conclusions: The formulation of fexofenadine hydrochloride 30 mg orally disintegratting tablet was initially built with taste-masked, short disintegrating time and high dissolution rate.

<PP-20>

Tolerogenic nanovaccine formulation in treatment of automatic disease

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Keywords: polydopamine, ovalbumin, dexamethasone, tolerogenic dendritic cell, antigen- specific immune tolerance

Background: An autoimmune disease arises when the immune system mistakenly targets the body instead of safeguarding it. Dexamethasone (DEX) has long been employed as a potent immunosuppressive agent in the treatment of inflammatory and autoimmune diseases, despite the occurrence of significant side effects. In this study, DEX and the model antigen ovalbumin (OVA) were encapsulated with polydopamine to specifically deliver DEX and OVA to dendritic cells, thereby mitigating the systemic side effects associated with DEX administration. The nanoparticles (NPs) exhibited a pronounced ability to induce immune tolerance towards OVA, leading to a favorable therapeutic outcome.
Methods: Development of nanostructured vaccines using a complexing mechanism facilitated by zinc ion bridging, with a focus on optimizing component ratios, investigating nanosystem size, and ensuring tolerability. The formulation's ingredient concentrations were determined using UV-VIS spectroscopy, HPLC, and bicinchoninic acid (BCA) assays. Drug release studies were conducted at pH levels relevant to the intended application using dialysis membrane. Flow cytometry was employed to simulate the adsorption capacity of both free antigenic proteins and antigenic proteins contained in nanoparticles into dendritic cells. Finally, the specific immunosuppressive effect of OVA antibodies was evaluated in mouse models using ELISA.
Results: PDA materials were synthesized under alkaline condition, enabling the successful formulation of a nanovaccine with exceptional stability and precise size control (average size of 150.2 nm). This nanovaccine exhibits the capability to release DSP in a pH-dependent manner, allowing for the mitigation of sudden drug release, and thus preventing the rapid elimination of DSP from the body. Such controlled release holds significant promise for extending the half-life of DSP at the site of injection (pH 7.4) and ensuring prompt release within the intracellular lysosome environment (pH 4.5). Moreover, the introduction of antigenic proteins in nanostructures results in more efficient uptake by dendritic cells compared to their free form. Evaluation of the nanovaccine in a mouse model further demonstrates its remarkable capacity to acquire an OVA specific immunosuppressive effect, evidenced by the elimination of anti-OVA antibodies of mice induced with OVA antigen.
Conclusions: These results suggest the applicability of nanovaccine as a potential drug delivery system and demonstrate of polydopamine NPs encapsulating both antigen and DSP is a useful means of inducing antigen-specific immune tolerance, which is crucial for the treatment of autoimmune diseases.

<PP-21>

Formulation and in vitro evaluation of film-coated tablets contaning sitagliptin and metformin hydrochloride 50/1000 mg

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Keywords: Sitagliptin monohydrate phosphate, metformin hydrochloride, film-coated tablets

Background: Diabetes mellitus is a dangerous chronic disease that cause many unpredictable comphication on heart, kidney and nerve, even causing death. Up to now, metformin is still first-line oral treament with many advantages. The combination of metformin with another agent such as dipeptidyl peptidase-4 inhibitor (sitagliptin) is now on study and developed. This study aims to prepare a formulation of film-coated contaning sitagliptin (as sitagliptin monohydrate phosphate form) and metformin hydrochloride 50/1000 mg.

Methods: Sitagliptin monohydrate phosphate and metformin hydrocholride high-dose 50/1000 mg film-coated tablets was prepared by wet granulation technique.The tablets is evaluate for thickness, weight variation, drug content and dissolution. In vitro release studies were also conduted to compare with the marketed product Janumet® 50/1000 mg, manufactured by Merck Sharp & Dohm.

Results: The optimal formulation of film-coated tablets containing 2.5% (w/w) of superdisintegrant presents well dissolution (98% in 30 minutes) and great tablet's properties. The in vitro behaviors of the research drug were equivalent to the brand name drug, Janumet® 50/1000 mg.

Conclusions: The film-coated tablets of sitagliptin and metformin hydrochloride can be alternative drug to candicate combination thepary treament in the commercial pharrmacy against diabetes mellitus.

Pharmacognosy & Natural Products

<PP-22>

The non-saponin fraction of Korean Red Ginseng suppresses muscle loss by maintaining immune homeostasis in old mice

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Keywords: Non-saponin faction of Korean Red Ginseng, muscle loss, sarcopenia, immune homeostasis, aging

Background: Muscle loss appears for a variety of reasons, especially aging, and when it gets worse, muscles abnormally reduced or weakened, leading to sarcopenia. Preventing sarcopenia, which has a high incidence in the elderly, is very important for improving their healthy physical activity and quality of life.
Methods: The non-saponin fraction (NSF) of Korean red ginseng is obtained by eliminating saponins from the red ginseng concentrate. We evaluated the muscle loss inhibition effect of NSF using 20-24-month-old C57BL/6 mice. Mice were orally administered NSF (50 or 200 mg/kg/day) daily for 6 weeks. After sacrifice, hindlimb muscles, thymus, and lymph node were cut out for further analysis.
Results: As results, NSF significantly increased muscle size in old mice. NSF normalized the size of the thymus and lymph node in old mice and recovered age-associated disturbance of immune homeostasis by retaining CD45+CD3+ cells.
Conclusions: In this study, we elucidated the close relationship between muscle loss and immune homeostasis and found that NSF inhibited severe muscle loss due to aging by maintaining immune homeostasis in old mice. Therefore, we propose the possibility that NSF could be used as a material for improving sarcopenia and immune homeostasis-maintaining functional foods for the elderly.

<PP-23>

Optimize steam distillation extraction and make care-hair gel with *Citrus maxima* peel essential oil

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Keywords: Citrus maxima, pomelo essential oil, steam distillation, care-hair gel

Background: Green chemistry with the trend of "circular, reuse," aims to protect the environment through the reuse of agricultural by-products. Pomelo (Citrus maxima), a tropical plant, is well-suited to Vietnam's climate and soil conditions and is identified as a major crop in many regions, including Dong Nai province. With the increasing cultivation area and yield of pomelo, the amount of waste generated by by-products (such as peels, seeds, and pruned young pomelo) poses a significant environmental issue. The current practice of dumping and landfilling is not sustainable. However, numerous studies have shown that pomelo peels contain valuable compounds with applications in various fields. For example, pomelo peel essential oil can be used in perfumery, aromatherapy, spirituality, and cosmetics. The process of extracting essential oil through steam distillation is suitable for economic feasibility and technical conditions and can be optimized. This extracted essential oil can then be formulated into a nourishing hair gel to utilize the grapefruit by-product to promote community health while addressing environmental challenges.
Methods: The full 2-level factorial design and central composite design of the response surface model in Design-Expert v13 software were employed to design and experiment, respectively, to find the main influential factors in the extraction process and to find optimal conditions for steam distillation extraction. The care-hair gel was formulated with a 10% concentration of pomelo peel essential oil. The wet gum method was used to emulsify the essential oil using a mixture of tween 20 and span 60 as the emulsifying agents. Subsequently, the gel was formed using carbomer 940 as the gelling agent.
Results: The optimized extraction process involved the following conditions: grinding time of 35 seconds, water-to-peel ratio of 2, extraction mixture volume-to-flask volume ratio of 0.75, boiling at 1400W power, and extraction time of 92.77 minutes. The extraction efficiency achieved was 0.91 ml/100 g of raw material. The formulated gel met the requirements for uniformity, gel consistency, skin pH, non-irritation, and stability during storage.
Conclusions: The experimental results can be practically implemented to utilize pomelo cultivation by-products as a raw material source for formulating healthcare products for humans while simultaneously addressing environmental issues.

<PP-24>

Semi-quantitative determination of the saponins in Vietnamese ginseng (*Panax vietnamensis,* Araliaceae*)* by thin-layer chromatography

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Keywords: Panax vietnamensis, saponin, thin layer chromatographic, majonoside R2

Background: Vietnamese Ginseng (*Panax vietnamensis*, Araliaceae – VG) is considered as National Wealth of Vietnam. The main composition of VG is the high content of protopanaxadiol, protopanaxatriol, and especially ocotillol-type saponins. The current quantitative method using HPLC-DAD is ineffective in detecting ocotillol-type saponin. The study's objective is to develop the semi-quantitative thin-layer chromatographic (TLC) analysis of the saponins in VG used as a cheap, rapid, and convenient method for quality control of VG.

Methods: Vietnamese Ginseng powder is extracted ultrasonically with methanol 80%. An aliquot of 10 µl of the extracts was applied to the TLC and developed by the mobile phase of *n*-butanol – water – acetic acid (4:5:1, upper layer). The spots were visualized by 10% sulfuric acid in ethanol followed by heating at 110 °C. The plate was then scanned into image files and processed using ImageJ and Image Lab software. The method was validated with the criteria of system compatibility, specificity, intraday and interday precision, and accuracy.

Results: Three main saponins G-Rg1, M-R2 and G-Rb1 were well separated in the chromatographic condition. The quantitative method showed good regressive between the concentration and the spot volume with the $R^2 > 0,95$; The accuracy reaches %RSD < 10%; The recovery rate is in the range of 80 – 120%; The method is applied quantitatively determination the saponin content in 15 samples of Vietnamese Ginseng. The result shows the average concentrations of G-Rg1, M-R2, and G-Rb1 are 3,77%, 7,35%, and 0,43%, respectively.

Conclusions: In conclusion, the study initially finds a simple, cheap, and rapid method that can simultaneously assess the saponins content of Vietnamese Ginseng, and contribute to preliminary quality control of this valuable medicinal plant in the market.

<PP-25>

Chemical constituents of *Radix Gomphandrae molis*

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Keywords: *Radix Gomphandrae tonkinesis*, iridoid, lignan

Background: *Gomphandrae molis* Merr. is an herbal remedy that has been traditionally used for its medicinal properties. It belongs to the *Gomphandrae* genus, which is a member of the Icacinaceae family. This plant is known for its ability to nourish the body, support spleen function, act as a diuretic, and stimulate milk production. However, there is limited research available on this plant. Therefore, the purpose of this study was to identify the chemical compounds present in Radix *Gomphandrae molis*.
Methods: Extraction: reflux extraction with ethanol 95%. Isolation by column chromatography, preparative HPLC and structure elucidation by NMR spectrum comparing to reference data.
Results: The study isolated some compounds belonging to lignan and iridoid groups. They are (+)-isolariciresinol 3α-O-β-glucopyranoside, (-)-isolariciresinol 3α-O-β-glucopyranoside, (+)-lyoniresinol-3α-O-β-glucopyranoside, (7R,8S)-dihydrodehydrodiconiferyl alcohol 9-O-β-glucopyranoside, hedyotol C 7″-O-β-D-glucopyranoside (lignan group) and cantleyoside-dimethyl-acetal, cantleyoside, sweroside**,** 6'-O-β-D-apiofuranosylsweroside , dipsanoside A, dipsanoside B, dipsaperine, loganin (iridoid group).
Conclusions: The study isolated 13 compounds from Radix *Gomphandrae molis* containing 5 lignans and 8 iridoids.

<PP-26>

Morphine dependence is attenuated by the treatment of *Panax ginseng* and *Polygalae radix* combination treatment in mice

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Keywords: morphine, drug abuse, microRNA, dependence

Background: As part of an ongoing efforts to alleviate morphine dependence, we screened for anti-narcotic effect of natural products through behavior experiment. In addition, microRNAs, small noncoding RNA molecules that regulate post-transcriptional gene expression, and various genes in the brain of morphine-addicted mice. *Polygalae radix* is the dried rhizome of *Polygala tenuifolia* Wild and is reported as tonic and neuroprotective substances.
Methods: We compared each treatment alone ginseng, polygalae radix, and a combination of the two in various ratios for morphine-induced dependence in mice. Mice were pretreated with ginseng, polygalae radix, and the those two in various ratios once a day, 30 minutes before the first morphine treatment, and then injected with morphine twice a day at 12-hour intervals for 9 days. Physical dependence was assessed using a naloxone-induced morphine withdrawal syndrome experiment.
Results: The number of naloxone-precipitated jumps was significantly suppressed by the combination treatment of a specific ratio rather than the single treatment of ginseng, and polygalae radix. In addition, through PCR and western blot experiments, it was confirmed that the combination of ginseng, and polygalae radix in a specific ratio decreased the morphine dependence.
Conclusions: Therefore, this study suggested that a specific combination of red ginseng and natural products is more effective as a potential treatment for morphine dependence than treatment alone.

<PP-27>

α-Glucosidase inhibitory potential of *Homonoia riparia*: Implications for diabetes mellitus intervention

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Keywords: *Homonoia riparia*, phenolic, *α*-glucosidase, diabetes mellitus

Background: Diabetes mellitus is a prevalent metabolic disorder requiring effective therapeutic approaches. *α*-Glucosidase inhibitors have emerged as potential targets for managing this condition. In this study, we investigated the inhibitory activity of the ethyl acetate (EtOAc) fraction derived from *Homonoia riparia* leaves on *α*-glucosidase, a key enzyme implicated in diabetes mellitus treatment.
Methods: The leaves of *H. riparia* were collected in Quang Ngai province, Vietnam, authenticated, and deposited in the Herbarium. The dried leaves were macerated with ethanol, and subsequent partitioning with *n*-hexane, ethyl acetate, and *n*-butanol yielded four fractions. Separation was achieved using column and thin-layer chromatography techniques. 1D-, 2D-NMR and ESI-MS spectra were recorded for compound characterization. The *α*-glucosidase inhibitory activity was evaluated using a modified assay with enzyme solution, sample solutions, and pNPG substrate. Absorbance measurements were taken at 405 nm, with acarbose as a positive control. Statistical analysis was conducted using the t-test and simple linear regression in Excel.
Results: In this study, the phytochemical analysis of the EtOAc fraction from *Homonoia riparia* led to the identification of five compounds: quercetin, myricetin, ethyl gallate, gallic acid, and myricitrin. The structures of these compounds were elucidated using spectroscopic methods such as MS, 1D-, and 2D-NMR, and by comparison with published data. Notably, this is the first report of these compounds being isolated from *H. riparia* leaves collected in Quang Ngai province, Vietnam. Evaluation of *α*-glucosidase inhibitory activity revealed that the EtOAc fraction exhibited the highest inhibitory potency, with an IC_{50} value of 1.763 µg/mL. These findings emphasize the potential of *H. riparia* as a source of *α*-glucosidase inhibitors and contribute to expanding the knowledge of its phytochemical composition.
Conclusions: The EtOAc fractions of *H. riparia* leaves showed potent bioactivity, including considerable *α*-glucosidase inhibition. Isolation of quercetin, myricetin, ethyl gallate, gallic acid, and myricitrin from these fractions highlights their bioactive potential and their first-time discovery in *H. riparia* leaves collected from Quang Ngai province, Vietnam. These findings underscore *H. riparia*'s potential as a natural source of *α*-glucosidase inhibitors for diabetes mellitus treatment.

<PP-28>

The anti-inflammatory activity of the extracts and compounds isolated from stems and leaves of *Dichroa febrifuga* Lour.

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Keywords: *Dichroa febrifuga*, Hydrangenoside C, Isoarborinol, Methyl 1,3,4,6-tetra-O-acetyl-fructofuranoside, anti-inflammation

Background: Inflammation is a remarkable problem in medicine, especially during the COVID-19 pandemic. *Dichroa febrifuga* Lour. is a traditional medicinal herb that has been applied in the treatment of malaria and some other infectious diseases. This study was conducted to investigate the anti-inflammatory activity of the extracts and compounds isolated from stems and leaves of *Dichroa febrifuga* Lour.
Methods: Stems and leaves of *D. febrifuga* were collected in Quang Nam province; then proceeded to extract, isolate, and determine the structure of the compounds. *In vivo* anti-inflammatory activity was evaluated using a carrageenan-induced mouse paw edema model on extracts and isolates. Compounds with good activity will be confirmed *in silico* using docking software to preliminary evaluate the anti-inflammatory mechanism.
Results: Three compounds including Hydrangenoside C (**1**), Isoarborinol (**2**), Methyl 1,3,4,6-tetra-O-acetyl-fructofuranoside (**3**) were isolated. *In vivo* tests showed that the extract had mild anti-inflammatory activity. Among 3 compounds, **2** significantly reduced the swelling similar with diclofenac. The activity of **2** was dose dependently. The docking result revealed that **2** could not form binding to COX-1 and COX-2 while having a high affinity for 5-LOX and PLA2 via generating hydrogen bonds.
Conclusions: This is the first study demonstrated that **2** isolated from *Dichroa febrifuga* Lour. significantly inhibited the inflammation using *in vivo* and *in silico* models. Further studies should be conducted to elucidate the promising bioactivities of this compound.

<PP-29>

Mechanisms of *Siegesbeckia orientalis* L against Gouty arthritis explored by network pharmacology combined with molecular docking

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Keywords: gouty arthritis, inflammation

Background: Gouty arthritis (GA) is a significant global public health concern due to its high prevalence. *Siegesbeckia orientalis* L (*S. orientalis*) has shown effectiveness in treating GA. However, the active compounds and their associated mechanisms of action remain unclear. This study aims to investigate the active compounds and the underlying pharmacological mechanisms of *S. orientalis* in the treatment of GA.
Methods: Initially, a network pharmacology approach was employed to identify the active compounds present in *S. orientalis*, as well as predict the potential targets and signaling pathways involved in its therapeutic effects. Subsequently, a molecular docking strategy was utilized to forecast the affinity between the active compounds and crucial targets.
Results: 8 active components and 20962 targets were identified, of which 460 targets were common targets for the drugs and diseases. 15,16-di-O-acetyldarutoside, hythiemoside B, pubeside C, stigmasterol, β-sitosterol, 3,7-O-dimethylquercetin, quercetin and ursolic acid, were identified as key active compounds. In PPI analysis, ATK1, HIF1A, IL1B, IL6, MAPK1, MAPK3, PTGS2, STAT3, TNF and VEGFA were screened out. GO enrichment analysis indicated that S. orientalis was likely to interfere with inflammatory response (GO:0006954) in the treatment of GA, and KEGG enrichment analysis indicated multiple inflammation-related signaling pathways possibly involved in the treatment of GA by *S. orientalis*, including TNF, HIF-1, and PI3K-Akt signaling pathways. The results of molecular docking indicated that the active compounds had good binding properties to their key targets.
Conclusions: In this study, we propose that *S. orientalis* possesses properties of multicomponent, multitarget, and multi-pathway activity in treating GA. Additionally, we aim to identify the key ingredients in *S. orientalis* and elucidate the interaction between these ingredients and their corresponding targets through relevant pathways. The potential ability of *S. orientalis* to alleviate GA may be attributed to its ability to inhibit inflammation.

<PP-30>

Cytotoxic compounds from *Hedyostis capitellata*

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Keywords: *Hedyotis capitellata*, sistosterol, triterpene, anthraquinone, cytotoxicity

Background: "Dạ cẩm" (*Hedyotis capitellata* Wall. ex. G. Don, Rubiaceae) has been used in folk medicine for stomach pain and for mouth ulcers. There is limited research available on this plant. The aim of this study is to explore the chemical constituents, as well as the cytotoxic activities of *H.capitellata*, in order to provide scientific evidence for the utilization and development of the product derived from this plant.
Methods: *Hedyotis capitellata* was collected at Thua Thien Hue province in March 2020. The plant material was percolated with 96% and 50% ethanol, then the crude extract was separated by liquid–liquid distribution. The isolation of pure compounds was conducted by column chromatography. The structures of isolated compounds were identified by MS, NMR spectroscopy methods. The cytotoxicity of the extracts and pure compounds was evaluated using the MTT assay with RD and MDA-MB-231 cell lines.
Results: The ethanolic extract of *H. capitellata* was partitioned with polarity ascending solvents to get *n*-hexane, chloroform, ethyl acetate, *n*-butanol and water fractions. Chloroform, *n*-hexan fractions showed the cytotoxic activity on RD cells with IC_{50} value of 47.66 ± 0.87 µg/ ml and 56,0 ± 1,59 µg/ ml, respectively. From the *n*-hexane extract, seven compounds were isolated and identified as: (**1**) sitostenone (21 mg), (**2**) stigmast-4-ene-3,6-dione (14.7 mg); (**3**) stigmastane-3,6-dione (22.2 mg), (**4**) 1-ethoxy, 2-methoxy anthracene-9,10-dione (14.7 mg), (**5**) 3-ethoxy-7-ol stigmast-4-ene, (**6**) acetyl ursolic acid (15.6 mg), (**7**) betulonic acid (15 mg). From the chloroform extract, three compounds were isolated and identified as: (**8**) ursolic acid (71mg), (**9**) pomolic acid (21 mg) and (**10**) scopoletin. Compound **2**, **4**, **7**, **8**, **9** showed the cytotoxicity activity in RD cell line with IC_{50} of the range 25,0 – 60,5 µM. Additionally, compound **6**-**9** inhibited the growth of MDA-MB-231 cell with IC_{50} values < 20 µM.
Conclusions: Triterpene and anthraquinone are the main compounds responsible for the cytotoxic activities of *H. capitellata* in cancer cell lines.

<PP-31>

Screening the hypouricemia effect of some Vietnamese remedies used for treating Bi syndrome in traditional medicine

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Keywords: xanthine oxidase, uric acid, Vietnamese remedies, Bi syndrome

Background: Hyperuricemia accounts for a high proportion of many populations. Although almost hyperuricemia cases are asymptomatic, current guidelines recommend conditionally start urate-lower therapy (ULT) when serum urate ≥ 9 mg/dl because of the increased risk for developing gout flares. The first-line drug of ULT is allopurinol – a xanthine oxidase (XO) inhibitor. However, allopurinol has many adverse effects. Many traditional remedies that treat Bi syndrome have been found to possess inhibit xanthine oxidase effect *in vitro* and/or hypouricemia effect *in vivo*. There are a lot of traditional Vietnamese remedies used to treat Bi syndrome, and some of the herbs in these remedies have been found to have XO inhibition activity. The aim of this study is to screen the *in vitro* hypouricemia effect of some Vietnamese remedies used for treating Bi syndrome.

Methods: Five remedies which met the suggested selection criteria from traditional Vietnamese books were chosen . The chosen remedies were extract with 70% ethanol (ratio of drugs : ethanol (g/ml) is 1:10). Preliminary screenings of chemical composition of medicinal extracts were performed by common chemical reactions. Extracts were tested for the XO inhibition *in vitro* by the procedure of Noro et al (1983) with some modifications.

Results: The chosen remedies include Thang tri te thap, Tho phuc que chi thang, Bai thuoc tru phong thap, Cao luong tru thap thang, and Bai nghiem phuong. Phytochemical screening showed the presence of flavonoids, saponins, alkaloids, tannins, and carbohydrates in all five extracts. At the concentration of 100 µg/ml, the percentage of XO inhibition of the remedies were 86.82 ± 4.78; 78.74 ± 2.24; 86.97 ± 1.74; 72,67 ± 7,36; and 8.73 ± 4.69%; respectively, while the inhibition proportion of allopurinol at the concentration of 0.075 µg/ml was 79.65 ± 0.93%. The IC_{50} of 4 former remedies were 48.33 ± 0.41; 60.34 ± 1.71; 50.31 ± 0.83; and 48.73 ± 8.99 µg/ml, respectively, while IC_{50} of allopurinol was 3.82 ± 0.25 µg/ml. The XO inhibition effect of these remedies may be related to the presence of flavonoids. The result of this study provided scientific evidence to consolidate the relevance between uric acid and “Dampness” syndrome in traditional medicine.

Conclusions: Phytochemical screening of the medicinal extracts showed the presence of flavonoids, saponins, alkaloids, tannins, and carbohydrates in all 5 remedies. Among 5 chosen remedies, 4 of them showed potential XO inhibitory effect, in which Thang tri te thap had the lowest IC_{50} value.

<PP-32>

Isolation of the active compound inhibiting microbial growth causing folliculitis from the ethanolic extract of noni fruit *Morinda citrifolia* L.

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Keywords: Folliculitis, Noni (*Morinda citrifolia* L.), Antimicrobial, Isolate, Scopoletin

Background: Folliculitis is a skin condition that is generally caused by microbes infection superficially or in hair follicles and forms pustules or erythematous papules on the skin covered by hair. People in their lives have used plants as one of the components that support the necessities of life and in certain cases, plants are used as a way to improve health because of easy and cheap access. One of the potential medicinal plants is the noni plant (*Morinda citrifolia* L.). Regarding the previous studies, *M. citrifolia* L. have antibacterial properties. This study aims to determine the active compound of noni fruit against the microbes that cause folliculitis.
Methods: Samples were extracted by maceration method using 96% ethanol as a solvent. Fractionation was carried out using a liquid-liquid extraction method with water, n-hexane, and ethyl acetate as solvents. Determining activity through quantitative and qualitative tests including disc diffusion test, TLC-bioautography test, and microdilution test. The most active fraction against *Staphylococcus aureus* ATCC 6538, *Pseudomonas aeruginosa* ATCC 9027, *Cutibacterium acnes* ATCC 11827 and *Candida albicans* ATCC 10231 was then further fractionated using the vacuum liquid chromatography method. The fraction containing the target compound was selected to proceed with purification using preparative TLC. Isolation characterization was carried out using a TLC scanner.
Results: The results showed that the ethanol extract of the noni fruit was more active than the ethanolic extract of the noni leaf with an effective concentration of 2.5-12.5 mg/disc against the bacteria *S. aureus*, *P. aeruginosa*, and *C. acnes* while the ethanol extract of the noni leaf was only active at a concentration of 12.5 mg/disc against the bacteria *C. acnes*. In addition, the ethyl acetate fraction exhibited stronger activity than the n-hexane fraction and the water fraction against the tested microbes. Compound S2 was isolated from the ethyl acetate fraction and was identified as scopoletin. In antimicrobial evaluation, scopoletin significantly inhibited the growth of *C. acnes* (MIC 1000 µg/mL) and *C. albicans* (MIC 250 µg/mL).
Conclusions: The presence of scopoletin indicates anti folliculitis-potency of *M. citrifolia* L., and might be promising candidates for natural antimicrobial agents, especially against *C. albicans*.

<PP-33>

Botanical characteristics, DNA barcode, preliminary screening of phytochemical constituents of *Paederia foetida* Linn., Rubiaceae

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Keywords: *Paederia foetida*, phytochemical constituents, DNA barcoding

Background: *Paederia foetida*, with the common name “Mơ lông", is a medicinal herb used to treat many diseases in the field of Traditional Medicine such as diarrhea, dysentery, or common in the daily diet of local people. However, not many documents related to morphology, anatomy, DNA barcoding of this species have been recorded or studied in Vietnam.
Methods: The samples collected from Botanical Garden at TDTU, were described the morphological and anatomical characteristics; analyzed the chloroplast DNA barcoding on ITS region. Preliminary phytochemical screening was conducted by improved Ciuley method. Moisture, total ash and extracted substance content were surveyed according to Vietnam Pharmacopoeia V standard.
Results: Mơ lông was identified as *Paederia foetida* Linn. based on morphological characteristics and DNA barcoding. Preliminary of phytochemical constituents and some purity criteria of the medicinal samples used are as follows. *Paederia foetida* contains: iridoids, essential oils, fats, free triterpenoids, flavonoids, cardiac glycosides, saponins. Some average values of the investigated indexes include: moisture (12,0217%), total ash (10,8575%), extractable content (alcohol solvent: 23,1375% with heat, water solvent: 43.4620 % with heat, 29.8556% without heat).
Conclusions: The study confirmed the scientific name of “Mơ lông” from Botanical Garden at TDTU is *Paederia foetida* Linn. (Rubiaceae) and determined preliminary of phytochemical constituents and some purity criteria of the medicinal samples used.

<PP-34>

α-glucosidase inhibitors from the stems of *Knema globularia*

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Keywords: *Knema globularia*, diabetes, α-glucosidase inhibitory activity

Background: *Knema globularia* (Lam.) Warb. has been used popularly as a folk medicine in the Asian region. Phytochemical analyses of this plant have revealed the presence of diverse scaffolds mostly isolated from the fruits and roots: flavonoids, polyketides, steroids, and lignans. However, there is a lack of phytochemical and pharmacological data on the stems of this plant. In addition, no report regarding the α-glucosidase inhibition of *K. globularia* extracts and isolated compounds has appeared.
Methods: Isolation and purification were performed on the bioactive fractions by using proper chromatographic methods, such as normal-phase silica gel column chromatography (CC), reversed-phase C_{18} CC, Sephadex LH-20, and using high-performance reversed-phase liquid chromatography (HPLC). The chemical structures were elucidated by an analysis of their NMR and high-resolution electrospray ionization mass spectrometry data as well as by comparison with literature values. The absolute configurations were determined using time dependent density functional theory electronic circular dichroism (TD-DFT-ECD).
Results: Ten compounds (**1**−**10**) were isolated from the stems of *K. globularia*. Globunones A−C (**1**−**3**) represent the initial combined structures of a flavan-3-ol core and a 1,4-benzoquinone core. Most compounds tested showed potent inhibition toward α-glucosidase with IC_{50} values in the range 0.4−26.6 μM. Calodenin A (**9**) was the most active compound with an IC50 value of 0.4 μM (the positive control, acarbose, IC_{50} 93.6 μM). A kinetic analysis of **9** revealed that it is a noncompetitive inhibitor.
Conclusions: This work enriches the information regarding the chemical diversity of the *K. globularia* plant and offers valuable guidance for synthesizing new compounds inspired by natural products that could be used as antidiabetic agents.

<PP-35>

A olean-type triterpenoid and a sterol isolated from the roots of *Parietaria debilis* G.Forst. Urticaceae

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Keywords: Sam dat Con Dao, *Parietaria debilis*, maslinic acid, daucosterol

Background: Sam dat Con Dao (*Parietaria debilis* G.Forst., Urticaceae) has long been used by people living in Con Dao as a type of Ginseng for the purpose of improving, enhancing health and preventing diseases. In Vietnam, there are currently not many research works on Sam dat Con Dao to clarify the active ingredients as well as biological effects of this precious medicinal plant. Therefore, this study was conducted with the aim of isolating and determining the structure of compounds in dichloromethane extract extracted from the roots of Sam dat Con Dao, as a premise for biological tests as well as standardization.

Methods: The roots of *Parietaria debilis* G.Forst., collected in Con Dao National Park in May, 2018. Plant material was macerated with ethanol 96%. The crude extract was separated by liquid liquid distribution. The isolations of pure compounds were carried out by different means of column chromatography (classical column chromatography, Sephadex chromatography). The structures of isolated compounds were identified by MS, NMR methods.

Results: Plant material was macerated with 96% ethanol. The ethanol extract was evaporated to a concentrated residue under reduced pressure, then dissolved in water and partitioned with polarity ascending solvents (*n*-hexane, dicloromethan, ethyl acetate, *n*-butanol) to yield 5 fractions. The dicloromethan and ethyl acetate fraction were separated by different means of chromatography to give two compounds: maslinic acid and daucosterol.

Conclusions: The chemical study of dicloromethan and ethyl acetate fraction extracted from the roots of *Parietaria debilis* G.Forst. led to the isolation of two compounds: maslinic acid and daucosterol. Thereby creating a premise for biological experiments as well as further studies on Sam dat Con Dao.

<PP-36>

Investigation of anti-inflammatory activity from extract and isolated compound in the aerial part of *Houttuynia cordata*

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Keywords: *Houttuynia cordata*, aristolactam BII, anti-inflammation, ligand docking

Background: *Houttuynia cordata* Thunb. belongs to the Saururaceae family, in addition to using the whole plant as a vegetable, is also used in folk medicine to treat. With its characteristic chemical constituents including volatile oils, alkaloids, flavonoids, and phenolic acids, *H. cordata* could be a potential candidate for research on pharmacological effects. Aristolactam BII is a compound found in *H. cordata.*
Methods: The *H.cordata* was extracted with methanol to create the *H. cordata* extract. From that, aristolactam BII was separated and obtained by using chromatography. A carrageenan-induced edema mouse model was performed to investigate the anti-inflammatory ability of the methanol extract and aristolactam BII. Lastly, a ligand docking experiment was performed to determine the binding free energy of aristolactam to inflammatory proteins.
Results: After being extracted with MeOH (3 times, 3.5 L each) at room temperature, 35g of *H. cordata* extract was collected. Obtained substance from *H. cordata* methanol extract was identified as aristolactam BII. The methanol extract exhibited moderate anti-inflammatory activity when the swelling reduction rate at 4 h compared with saline was close to 20%. Reducing inflammation slightly but the difference was not statistically significant ($p > 0.05$). On the other hand, aristolactam effectively reduced the swelling after 4h ($p<0.05$) and 5h ($p<0.01$). Mice given diclofenac experienced a comparable outcome. ($p<0.05$). When conducting ligand docking, aristolactam BII was found effectively bound to both COX-1 and COX-2 with low energy (-56.5 and -51.5 kcal/mol). The energy is even lower compared to that of diclofenac (-24.63 and -34.82 kcal/mol).
Conclusions: *Houttuynia cordata* Thunb. is an herbaceous plant which showed diverse activities. The results showed that the extract inhibited the intensity of edema weaker than diclofenac, although paw volume was still reduced and visible. On the other hand, aristolactam BII had a stronger edematous effect than the positive control. The *in silico* research demonstrated that the anti-inflammation activity of aristolactam BII may be mediated by inhibiting COX-1 via generating h-bonds at the positions of Arg 120, Ser 530 residues and COX-2 via Ser 530 and Trp 387. Taken together, this revealed that the *H. cordata* methanol extract and the aristolactam BII compound isolated from that might have the anti-inflammatory function.

<PP-37>

Discovery of novel nucleoside, purine derivatives from the sponge species *Petrosia* sp. in Phu Quoc island

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Keywords: nucleoside, purine, *Petrosia* sp.

Background: Marine sponges, classified under the phylum Porifera, are some of the earliest and most basic creatures on Earth. They thrive in all oceans and possess remarkable resilience to cope with extreme temperatures and pressures. The sponge has non-specific cells that can transform into other types of cells and that often move between the primary and mesohyl cell layers. Furthermore, these sponge species are renowned for their ability to produce secondary metabolites, which serve as an effective defense mechanism against external predators. The compounds isolated from the sponges of this genus, *Petrosia* have quite significant activity such as anti-inflammatory, antioxidant, immunomodulatory, anti-infection, antibacterial, and especially inhibiting the HIV virus. In this study, a novel nucleoside (thymipetrosia) (**1**) and purine (azapetrosia) (**2**) were isolated by towards bioactivity.
Methods: On the preliminary three sponge species screening, including *Clathria reinwardti*, *Xestospongia testudinaria*, and *Petrosia* sp., we observed that the extracts of *Petrosia* sp. exhibited the highest antibacterial and cytotoxicity activity as determined by the brine-shrimp testing, MTT, and broth microdilution assay. The extracts displaying promising bioactivity underwent open-column chromatography to isolate pure compounds. Their chemical structures were elucidated based on extensive spectroscopic analyses, including NMR, HR-ESI-MS, HR-ESI-MS/MS, ESI-MS, IR, UV, and comparisons with published data.

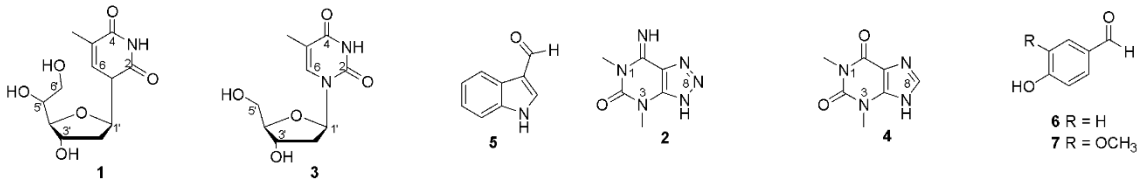

Figure 1. Structures of isolated compounds (**1-7**) from *Petrosia* sp.

Results: The sponge *Petrosia* sp. was the best inhibitor of *Artemia salina* (LC_{50} ranging from 6.09 to 147.63 µg/mL), and KB cells (IC_{50} from 88.73±4.21 to 326.19±8.95 µg/mL). Moreover, testing for microorganisms, 3 out of 4 samples of *Petrosia* sp., were well inhibited by both Gram-positive (*Staphyloccocus aureus*, *Bacillus subtilis*, *Lactobacillus fermentum*) and Gram-negative (*Escherichia coli*, *Salmonella enterica*, *Pseudomonas aeruginosa*) bacteria species; that are the ethanol, ethanol/water, and dichloromethane extracts, with IC_{50} less than 40 µg/mL and MIC ranging from 16 to 250 µg/mL. From the ethanol extract, two new compounds thymipetrosia (**1**), azapetrosia (**2**), and five known compounds, including thymidine (**3**), theophylline (**4**), 1*H*-indol-3-carbaldehyde (**5**), 4-hydroxybenzaldehyde (**6**), 4-hydroxy-3-methoxybenzaldehyde (**7**) were isolated and identified.
Conclusions: From the marine sponge *Petrosia* sp., a novel nucleoside (thymipetrosia) (**1**), purine (azapetrosia) (**2**), and five known compounds (**3-7**) were successfully isolated. Besides, sponge *Petrosia* sp. exhibited the strong cytotoxicity and antibacterial activities. Notably, both the ethanol extract and the ethanol/water extract of *Petrosia* sp. demonstrated significant inhibition against *Escherichia coli* bacteria (MIC = 16 µg/mL), which is comparable to the control Cefotaxime (MIC = 16 µg/mL).

<PP-38>

Bioassay-guided isolation anti-inflammatory effects of active compounds from the agarwood of *Aquilaria crassna*

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Keywords: *Aquilaria crassna*, phenylethylchromone, sesquiterpene, anti-inflammatory effect

Background: *Aquilaria crassna* Pierre (Thymelaeaceae) is widely distributed in Vietnam and has been used in traditional medicine for the treatment of insomnia, anxiety, asthma, cold, analgesic, and digestive disorders. However, the phytochemical and pharmacological studies on the agarwood of *A. crassna* were limited in Vietnam.
Methods: The agarwood chips of *A. crassna* (4.0 kg) were purchased from Evergreen Forest JSC. (Ho Chi Minh city, Vietnam) in December 2019. The raw materials were sonicated at 50 °C with 70% MeOH, the solvent evaporated under reduced pressure, then the MeOH extract was successively partitioned with increasing polarity of solvents. The structures of isolated compounds were elucidated by spectroscopic methods including UV, HRESI-MS, 1D and 2D-NMR. The extracts and compounds were evaluated for their inhibitory effects against LPS-induced NO production on BV2 cells at the tested concentrations of 1-50 µg/mL for the extracts and 1-50 µM/mL for the compounds.
Results: The extracts and compounds did not show any cytotoxicity at the tested concentrations. The *n*-hexane and ethyl acetate extracts showed the significant inhibition NO production in a dose-dependent manner with IC_{50} at 5.67 ± 0.9 and 26.46 ± 6.12 µg/mL, respectively. Nineteen compounds including phenylethylchromone and sesquiterpene derivatives were isolated from the ethyl acetate extracts. Among them, 6-hydroxy-2-[2-(4'-methoxyphenyl)ethyl]chromone showed significantly decreasing the levels of NO production on LPS-activated BV2 cells with IC_{50} value of 29.88 ± 8.2 µM when compared with positive control, quercetin (IC_{50} 7.28 ± 1.32 µM).
Conclusions: The *n*-hexane and ethyl acetate extracts, and the tested compounds showed moderate anti-inflammatory effects against NO production in BV2 microglial cells. To our best knowledge, ten compounds were first reported from the agarwood of *A. crassna*.

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Pharmaceutical Biotechnology

<PP-39>

The potential application of black shallot, a novel product of shallot (*Allium ascalonicum*), in terms of protection against alcoholic related liver injury

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Keywords: black shallot, hepatoprotective effect, polyphenols, antioxidant activity

Background: Black shallot is a new food product on the market today that is derived from shallot (*Allium ascalonicum*) under the aging process in high temperature. It is a potentially healthy food, but there is still not much research about its bioactivity and production process.
Methods: In this study, we investigated the changes of polyphenol content (using Folin Ciocalteu reagent) and of antioxidant activity (through DPPH radical scavenging assay) of black shallot during incubation process at 3 different temperatures (60°C, 70°C, 80°C). From these results, we chose optimal conditions for production of black shallot. Then the optimal product was used to evaluate the protection effect of black shallot against liver injuries which was established via oral administration of ethanol (30 mL of 28.5% ethanol/kg B.W. for 30 days). The liver injury severity was assessed via blood biochemical testing (ALT, AST, LDH) as well as histological analysis.
Results: We found that polyphenol content and antioxidant activity of black shallot produced at 70°C for 18 days was the highest value. Therefore, we chose this condition to produce black shallot. Furthermore, when we treated the mice with black shallot, black shallot not only ameliorated biochemical parameters (AST, ALT, LDH) in system level but also reduced the inflammation signs in histological level.
Conclusions: From these data, it indicated that black shallot can be a functional food with high potential in the future to be applied in food and pharmaceutical industries.

<PP-40>

Antioxidant and skin anti-aging effects of *Rourea oligophlebia* Merr. root extracts on HaCaT keratinocytes

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Keywords: Antioxidant, Anti-skin aging, HaCaT cell lines, *Rourea oligophlebia* Merr.

Background: *Rourea oligophlebia* Merr. species belongs to the genus *Rourea*. This species is a medicinal plant that has been traditionally used for bleeding, bone fracture treatments, and stress relief. It contains flavonoids, coumarins, triterpenes, lipids, and phenolic acids with good biological activities. This study aims to evaluate the antioxidant and anti-skin aging activities of the *n*-hexane, EtOAc, *n*-BuOH, MeOH, and aqueous extracts from the roots.
Methods: The antioxidant capacity was examined by reducing power, ferric-reducing antioxidant power, and $ABTS^{\bullet+}$ radical cation assays. The total phenolic and flavonoid contents (TPC and TFC) were determined using Folin-Ciocalteu and $AlCl_3$ colorimetric assays. MTT survival assay and Western blot analysis were used to investigate the anti-skin-aging activity on HaCaT keratinocytes.
Results: All extracts potentially exhibited antioxidant activity with IC_{50} values ranging from 2.93 to 5.73 µg/mL for $ABTS^{\bullet+}$ except the *n*-hexane extract due to their high TPC values. Moreover, the *n*-BuOH, MeOH, and aqueous extract possess promising anti-skin aging activities, as observed by attenuation of UV-A toxicity on human keratinocytes. We proposed that these anti-skin aging properties are possibly due to direct scavenging activity against reactive oxygen species and upregulate cellular antioxidant machinery.
Conclusions: To the best of our knowledge, it was the first report to demonstrate the antioxidant and anti-skin aging activities of the extracts of *R. oligophlebia* roots. The results indicated that this species could be a potential source of natural antioxidants and anti-aging. Consequently, it can be further investigated as a medicinal plant that assists in prescribing oriental traditional uses.

<PP-41>

Hopan-type triterpenoids from the thallus of lichen *Parmotrema tinctorum* (Despr. ex Nyl.) Hale

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Keywords: lichen, *Parmotrema tinctorum*, hopan-triterpenoid

Background: Lichens are symbiotic organisms of mycobionts and fungi with an abundance of bioactivity, proven by folk medicine and modern research. Previous chemical investigations of lichens have reported several kinds of compounds, which were unique in the genus lichen. Up to now, only a few publications related to triterpenoids of *Parmotrema tinctorum* have been reported. Herein, we report the separation and elucidation of three hopane-type triterpenoids including a novel peracid, tinctoride A (**1**), along with two known compounds zeorin (**2**), 6*β*,22-dihydroxyhopane (**3**) from the ethyl acetate extract of *P. tinctorum*.
Methods: These compounds were isolated by chromatography (Sephadex LH-20, TLC, and normal and reversed-phase) from the ethyl acetate extract of the lichen *P. tinctorum* collected in Lam Dong province. The chemical structure was elucidated by NMR spectra (1D and 2D), HRESIMS, IR spectra and comparison with those reported in the literature.
Results: Compound **1** was obtained as a white amorphous powder with the molecular formula of $C_{34}H_{54}O_7$, as deduced from the ion peak in HRESIMS. The characteristic proton and carbon signal of **1** suggested that **1** was a hopane-type triterpenoid with two acetoxycarbonyl groups at C-1 and C-3, further supported by HMBC correlations of H-1 (δ_H 4.66) to C-31 and H-3 (δ_H 4.58) to C-33. Moreover, the presence of peracid moiety located at C-30 was clearly evidenced by the FT-IR spectrum and chemical shift of C-30 (δ_C 181.9) instead of 184 ppm in the case of acid function. The relative stereochemistry of 1 was determined by pair-to-pair NOESY interactions. Altogether, the chemical structure of **1** was elucidated as 1*β*,3*β*-diacetoxy-21α-hopan-29-oic peracid, namely tintoride A.
Compound **1**-**3** were evaluated for their alpha-glucosidase. Compound **2** showed weak inhibition (IC_{50} 258.87 μM) and no inhibition for compounds **1** and **3**, compared to positive control, acarbose (IC_{50} 108.08 μM)

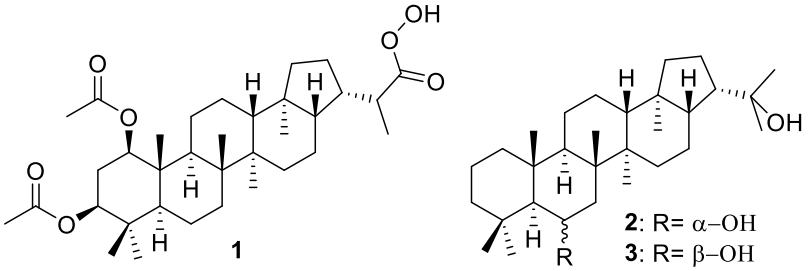

Figure. Chemical structure of compounds **1**-**3.**

Conclusions:
Three hopan-type terpenoids including one novel peracid, tinctoride A, and two knowns, zeorin (**2**) and 6β,22-dihydroxyhopane (**3**) were identified from the lichen *P. tinctorum.* Three compounds displayed null or weak inhibitory activity against *α*-glucosidase.

<PP-42>

Searching for AchE inhibitors from natural compounds by using machine learning and atomistic simulations

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Keywords: AChE, alzheimer's disease, docking, FPL, Machine learning

Background: Acetylcholinesterase (AChE) is one of the most important drug targets for Alzheimer's disease treatment. In this work, a combined approach involving a Machine Learning model and atomistic simulations was established to predict the ligand-binding affinity to AChE. GraphConv model was selected and utilized to rapidly and accurately screen the natural compound database for potential AchE inhibitors.
Methods: The four main methods used in the research are computational Machine Learning combined with atomic simulations including docking simulation and steeredmolecular dynamics simulations to find out the binding affinity of compounds with AChE, investigated pharmacokinetic parameters including blood-brain barrier ability and toxicity of compounds to select the most optimal compound.
Results: Good agreement between ML and atomistic simulations was observed. Twenty compounds were suggested to be able to inhibit AChE. Especially, four of them including geranylgeranyl diphosphate, 2-phosphoglyceric acid, and 2-carboxy-d-arabinitol 1-phosphate, and farnesyl diphosphate are highly potent inhibitors with sub-nanomolar affinities. These compounds with log(BB) in the range of −0.59 to 0.00 were able to cross the blood-brain barrier. Moreover, the hERG inhibition index showed that these compounds could not have toxicity to the human body.
Conclusions: In this work, a combined ML/FPL approach was proposed to predict the binding affinity of a ligand to AchE. Overall, our obtained results may stimulate the search potentials drugs for an Alzheimer's disease therapy.

Pharmaceutical Analysis & Quality Control

<PP-43>

Identification of eleven medicinal herbs in the capsule product treating thrombosis, angina by thin layer chromatography method

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Keywords: Identification, medicinal herbs, traditional Chinese medicine, TLC method

Background: *Xuefu Zhuyu* is a famous remedy of traditional Chinese medicine used for the treatment of cardiovascular diseases such as thrombosis, angina. To meet treatment needs nowadays, a capsule product has been manufactured with the formulation basing on this remedy including eleven medicinal herbs: *Semen Persicae, Flos Carthami tinctorii, Radix Angelicae sinensis, Rhizoma Ligustici wallichii, Radix Paeoniae, Radix Bupleuri, Radix Rehmanniae glutinosae, Fructus Aurantii, Radix Platycodi grandiflori, Radix Achyranthis bidentatae, Radix Glycyrrhizae*. Initially, the medicinal herbs were extracted with ethanol 50%. After that, the extract was concentrated to the specified moisture before being mixed with excipients and packed into capsules. The TLC method was used to identify the presence of the eleven herbs in this capsule product quickly, which contributed to improve the drug quality control.

Methods: Reference medicinal herbs and the drug powder were extracted with the same suitable solvents. Then, the extracts were concentrated to about 2 milliliters before being dotted on TLC silica gel F_{254} plates and carried out chromatographically with appropriate mobile phases. After chromatography development, spots were detected by placing TLC plates under ultraviolet light or by spraying appropriate reagents.

Results: *Radix Angelica sinensis, Rhizoma Ligustici wallichii* were extracted with n-hexan, the mobile phase was n-hexan - ethyl acetate (9:1), spots were detected by placing TLC plates under ultraviolet light of 365 nm. *Fructus Aurantii, Flos Carthami tinctorii* were extracted with ethyl acetate, the mobile phase were chloroform - methanol - water - acetic acid (13:4:1:1,5) and ethyl acetate - formic acid - acetic acid - water (15:1:1:2) respectively, spots were detected by spraying the solution of $AlCl_3$ 1% then placing TLC plates under ultraviolet light of 365 nm. *Radix Paeoniae* was extracted with acetone, *Semen Pruni* was extracted with methanol, *Radix et Rhizoma Glycyrrhizae, Radix Bupleuri chinensis, Radix Platycodi grandiflori, Radix Achyranthis bidentatae, Radix Rhemanniae glutinosae* were extracted with n-butanol, mobile phases were acetone - ethyl acetate - acetic acid (3:7:0,5), toluen - ethyl acetate (5:5), ethyl acetate - formic acid - acetic acid - water (15:1:1:2), chloroform - methanol - water (13:4:0,5), chloroform - methanol - acetic acid - water (8:1,5:4:1), chloroform - methanol - water - formic acid (8:5:1:0,2), chloroform - methanol - acid acetic (10:1,5:0,1) respectively, spots were detected by spraying the vanilin/sulfuric acid reagent and heating.

Conclusions: The solvents that were used to extracted were selected suitably with group compounds contained in herbs. *Radix Angelica sinensis* and Rhizoma *Ligustici wallichii* were carried out chromatographically with the same mobile phase because they contain the quite similar compounds, while the other nine herbs were conducted with nine different mobile phases.

<PP-44>

Determination of vitamin C in multivitamin gummy candies for children by HPLC - PDA method

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Keywords: Determination, vitamin C, multivitamin, HPLC method

Background: Vitamin C is one of the essential vitamins that is responsible for a wide range of important functions in human bodies. However, humans have lost the ability to synthesize vitamin C on our own in the evolutionary process. Therefore, we have to supplement vitamin C from external sources to prevent deficiency of this vitamin. Nowadays, the multivitamin gummy candy is one of the commonly used products to provide vitamin C for children because of its convenience. While gummy candies supplying vitamin C are increasingly being produced, determining vitamin C content in these products is necessary to ensure that the amount of this vitamin being given for children is appropriate. This study provides a process determining vitamin C in gummies rapidly and reliably by using HPLC - PDA method.

Methods: *Standard solution*: Dissolve vitamin C with a mixture of methanol - phosphoric acid solution pH 2.0 (5:95) to obtain a solution containing vitamin C with a concentration of 20 µg/mL, filter through a 0.45 µm filter, and inject immediately into the HPLC - PDA system.

Sample solution: A weight of gummies corresponding to 20 mg of vitamin C was dissolved with 40 mL of a mixture of methanol - phosphoric acid solution pH 2.0 (5:95) in a beaker by ultrasonic waves, transfer the entire solution to a 100 mL volumetric flask and fill to the mark with the same solvent. Accurately aspirate 5 mL of the resulting solution, dilute to 50 mL with the same solvent. Filter through a 0.45 µm filter and inject immediately into the HPLC - PDA system.

Investigating chromatographic conditions of HPLC - PDA such as chromatographic column, column temperature, detection wavelength, flow rate, sample injection volume, mobile phase to separate vitamin C peak meeting the requirements of resolution, symmetry factor, and peak purity.

Results: The optimal chromatographic conditions obtained are as follows: A mobile phase of a mixture of methanol - phosphoric acid solution pH 2.0 (5 : 95), column Phenomenex Gemini C_{18} (250 × 4.6 mm; 5 µm), column temperature at 20 °C, photo diode array detector is set at 243 nm, flow rate at 1.0 mL/min, injective volume is 20 µL. The established process was validated according to the guideline of the ICH 2005 - Q2 (R1) and showed the satisfaction of system suitability, specificity, linearity within 8.0 - 32.0 µg/mL ($y = 32.554x - 32.074$; $R^2 = 0.9994$), repeatability (RSD = 1.8%), intermediate precision (RSD = 1.1%), accuracy with recovery rates were from 99.4% to 99.7%, and the range of 12.0 - 28.0 µg/mL.

Conclusions: In the study, a rapid and reliable analytical process for determination of vitamin C in multivitamin gummy candies was developed by using HPLC - PDA method. The study's results would contribute to improve these products' quality control.

<PP-45>

In silico docking analysis of big structures from natural products

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Keywords: docking analysis, *in silico*, natural products

Background: The current study elucidates the molecular recognition mechanisms of immune receptors for common structures in big structures from natural products. By searching for big structures from natural products and other sources, we have identified the binding sites of big structures from natural products to immune receptors. It would contribute to the development of novel agents based on natural big structures from natural products.
Methods: Main experiments were to investigate how immune receptor recognizes common structures present in big structures from natural products. After conducting a literature search, we discovered that certain structures among these big structures from natural products are related to immunity.
Results: Through *in silico* docking analysis, we discovered that unique segments possess affinities for immunity, and our experiments demonstrated that big structures from natural products induce immune receptors.
Conclusions: Using recent docking analysis techniques, we unraveled the binding moiety to immune receptors, contributing to the development of new drug candidates based on natural big structures.

<PP-46>

Developing a quantitative HPLC method for the simultaneous determination of multi-saponins in *Panax vietnamensis* by a single reference standard

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Keywords: HPLC, *Panax vietnamensis*, simultaneous, single reference standard

Background: In the practice of comprehensive quality control of herbal medicine, the traditional method of choosing one marker for testing has gradually been replaced with the determination of multiple active components based on the synergistic interactions of herbal medicine and the applicability of advanced analytical techniques. However, a significant obstacle to achieving the goal has been the restricted availability of different reference substances for quantitative analysis given the abundance of herbal medicine on the market and their even more complex preparation. Single Standard for the Determination of Multiple Components (SSMDC) method, a novel technique to reflect the internal quality of herbal medicine, was proposed and adopted as a solution to these escalating issues.
Methods: In this study, SSMDC method is developed for quality control of Vietnamese Ginseng (*Panax vietnamensis*) by HPLC-PDA-ELSD. Consequently, conversion factors were established with each detector, and 5 saponins were determined, with only G-Rb_1 was single standard, or in some cases, there were G-Rb_1 and M-R2. The validation of determination, and validation of the factors affecting the conversion factors (ruggedness and robustness), were also conducted.
Results: The average conversion factors (F_{tb}) were established for G-Rb_1, G-Rd, G-Rg_1 and M-R2 (1.0000; 1.0845; 1.3195; 0.0367, respectively) in HPLC - PDA, and in HPLC - ELSD were 1.0000 (G-Rb_1), 0.9548 (G-Rg_1); 0.9201 (M-R2); 0.9701 (V-R2).
Conclusions: From the results, it can be seen that the difference when quantifying saponins in samples of Vietnamese Ginseng by F_{tb} and $F_{one\ day}$ is at an acceptable level (|SMD| ≤ 5.0 %).

Multimodality Drug Development

<PP-47>

Preparation of mesoporous silica nanoparticles

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Keywords: nanoparticles, mesoporous, silica

Mesoporous silica nanoparticles (MSNs) have become the innovation in material science to develop nanotechnology-based delivery systems. MSNs have widely applied in catalysis, biomedical, diagnostic, targeted therapy... Therefore, this study was focused on the synthesis of MSNs by the modified Stöber method. Tetraethyl orthosilicate (TEOS) was used as precursor of silica, and cetyltrimethylammonium bromide (CTAB) was used as pore generating agent.

The stability of vitamin E and paclitaxel on MSNs were investigated. Both of APIs are belong to group IV in the biopharmaceutical classification (poorly soluble and poor permeability).

The influencing factors on the properties of MSNs were investigated such as the molar ratio of CTAB/TEOS, the ratio of ethanol/water, reaction temperature, and reaction time. The silica particles were characterized by morphology (SEM), average particle size (DLS, SEM), pore size, specific surface area and total pore volume (N_2 adsorption isotherms – desorption isotherms with BET, BJH method), zeta - potential, structure determination (XRD)... The quantification of MSNs-API was developed and validated. Finally, the stability of MSNs-API was carried out at 40 ± 2 ºC, 75 ± 5% RH for 6 weeks.

MSNs were obtained with the moderate size and homogeneous (281.1 ± 1.960 nm, PdI: 0.265 ± 0.017), the pore size was about 3.864 nm, the surface area and pore volume were about 253.512 (m^2/ g) and 0.245 (cm^3/ g), respectively.

The entrapment efficiency of vitamin E and paclitaxel were 59.572 ± 0.25%, and 23.966 ± 0.606, respectively. Finally, the results showed that MSNs-API were stable at 40 ± 2 ºC, 75 ± 5% RH for 6 weeks.

The mesoporous nano silica materials were prepared successfully and proposed the method of loading API into MSNs such as vitamin E and paclitaxel.

<PP-48>

Study on renoprotective effect of Vietnamese ginseng (*Panax vietnamensis* Ha et Grushv., Araliaceae) to prevent Cyclosporine A-induced nephrotoxicity in LLC-PK1 cell line

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Keywords: Vietnamese ginseng, processed Vietnamese ginseng, nephroprotective, cyclosporin A

Background: Cyclosporine A (CsA) is an immunosuppressive agent that is used to prevent transplant rejection or treat autoimmune diseases. However, its clinical applications has been limited by severe adverse effects, particularly nephrotoxicity. This study aimed to investigate the protective effect of Vietnamese ginseng (VG) on CsA-induced nephrotoxicity in LLC-PK1 cell line.
Methods: LLC-PK1 cells were cultured in MEM medium media supplemented with 10% fetal bovine serum (FBS) and 1% penicillin/streptomycin under a humidified atmosphere with 5% CO_2 at 37°C. Cells were treated with CsA at concentrations 5 – 50 µM for 24, 48, 72 hours at densities 1.5; 3.0; 4.5 x 10^4 cells/cm^2, evaluated cell proliferation (MTT test), necrosis (LDH test), oxidative stress (cellular glutathione content) to choose suitable conditions. Raw and processed total extracts (RVG, PVG), crude saponin fractions (RS, PS), majonoside R2, and its ocotillol aglycon from VG were evaluated for nephroprotective effect to prevent cyclosporine A-induced nephrotoxicity in LLC-PK1 cell line.
Results: CsA reduced 36.3% of the cell viability at the dose of 15 µM after 48 hours of treatment, cell density of 3.0 x 10^4 cells/cm^2, compared to control group. Co-treatment of VG's samples with CsA could reverse the loss of cell viability in the range of 18 – 52%. Both PVG and PS at doses of 100 and 200 µg/mL could significantly decrease CsA-induced cell necrosis (48 – 84%), while the effect of RVG and RS showed at dose of 200 µg/mL. CsA could deplete 37.5% GSH content in LLC-PK1 cells. PVG, PS at doses of 100 and 200 µg/mL and RVG, RVS at dose of 200 µg/mL enhanced GSH levels with efficiency of 54 – 217%.
Conclusions: All the total extract and crude saponin fraction of raw and processed VG showed the nephroprotective effect against the injury induced by CsA. The results suggested that Vietnamese ginseng could be applied for prevention and/or treatment of CsA-induced nephrotoxicity.

<PP-49>

Comparative analysis of essential oils of Vietnamese ginsengs from dissimilar origins based on GC-MS based metabolomics approach

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Keywords: Vietnamese Ginseng, essential oils, GC-MS, metabolomic

Background: Vietnamese Ginseng is a precious medicinal herb, the saponin composition of Vietnamese Ginseng has been investigated in previous studies while almost no reports on its other non-saponin compounds. This study aims to compare the chemical composition of Vietnamese Ginseng essential oil cultivated in different regions and thus established a model for distinguishing VG from dissimilar regions based on its essential oil profiling.
Methods: Vietnamese Ginseng was purchased in Kon Tum and Lam Dong province. Then essential oils are extracted by the Soxhlet extraction method combined with the water distillation method. Analysis of essential was performed by gas chromatography-mass spectrometry (GC/MS). To analyze how geographical factors affect the chemical composition of essential oils, the relationship of essential oil composition between sample group was analyzed by principal component analysis (PCA) method and by the method of principal component analysis (PCA) and partial least squares-discriminant Analysis (PLS-DA).
Results: 111 components were identified in the essential oil of Vietnamese Ginseng grown in Kon Tum, the compounds with the highest content were: Falcarinol (29.66%), n-Hexadecanoic acid (13.8%), 9,12-Octadecadienoic acid (Z,Z)- (12.12 %). 93 components were identified in the essential oil of Vietnamese Ginseng grown in Lam Dong province, the main compounds were identified as: Falcarinol (21.33%), n-Hexadecanoic acid (13.49%), 9, 9, 12-Octadecadienoic acid (Z, Z)- (9.19 %),… the difference in composition of Vietnamese Ginseng essential oil when cultivated in different regions is clearly shown in the 2D score chart (PC1 vs. with PC2) of PCA and PLS-DA. 35 chemical compounds were identified as markers, contributing the most to the difference in composition of essential oil of Vietnamese Ginseng grown in Kon Tum compared with that in Lam Dong.
Conclusions: Vietnamese ginseng grown in different regions can lead to differences in essential oil composition. Identified chemical compounds, especially markers of 2 groups of essential oils, can be useful in tracing the geographical origin of Vietnamese Ginseng.

<PP-50>

Design and evaluating the efficacy of novel antibodies enhancing binding on CTLA-4 and PD-1 immune checkpoints

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Keywords: immune checkpoint proteins, CTLA-4, PD-1, protein-protein docking, alanine scanning

Background: Immune checkpoint proteins, including CTLA-4 and PD-1, have emerged as promising targets for cancer immunotherapy due to their vital role in immune regulation.
Methods: In this comprehensive study, we conducted a thorough analysis of antibody-protein interactions by employing structural analysis, mutational studies, and antibody-antigen docking simulations.
Results: Our findings revealed that antibodies **1** and **2** exhibited strong binding affinities towards CTLA-4 and PD-1 proteins, respectively. Further analysis through alanine scanning identified specific residues, namely Tyr91 on antibody **1**, as well as Asn31 and Asp96 on antibody **2**, as potential mutation sites. Introducing these mutations resulted in the generation of two novel antibodies, **1a**, **2a** and **2b**, which displayed enhanced binding affinity towards their respective target proteins.
Conclusions: With their improved binding capabilities, these novel antibodies hold tremendous promise for enhancing the effectiveness of antibody-based therapies designed to target immune checkpoints in cancer treatment. The ultimate objective is to significantly improve the health outcomes of patients by leveraging the potential of these novel antibodies.

<PP-51>

Investigation of alpha-glucosidase inhibitory effect of aqueous extract from flora *Hibiscus rosa-sinensis* L.

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Keywords: *Hibiscus rosa-sinensis*, alpha – glucosidase, diabetes, flower

Background: *Hibiscus rosa-sinensis* L. is a glabrous shrub, widely distributed in Vietnam. Aqueous extract of flora *H.rosa-sinensis* contains flavonoids such as quercetin, kaempferol, cyanidin-3,5-diglucoside, cyanidin-3-sophoroside-3-glucoside, alkaloids, mucilage and vitamins... In folk medicine, flora *H.rosa-sinensis* is used control blood sugar, treat dyslipidemia, treat inflammation of the lining of the stomach-intestines, bloody stools, dysentery, insomnia, pimple, itching, swelling. In addition, *H. rosa-sinensis* is also used to soothe dysmenorrhea, stimulate placental discharge after birth, treat cough, sore throat, treat gonorrhea in other countries.

Methods: Root, stem, leaf was stained with Carmine Alum, powder of flora and leaves in microscope. Preliminary phytochemical screening of aqueous extract from flora *H.rosa-sinensis* was conducted by improved Ciulei method and investigation of alpha-glucosidase inhibitory effect (Dai Thi Xuan Trang et al., 2012).

Results:

H. rosa-sinensis is identified based on the results of microscopic characteristics, especially in the stem, phloem fibers put together in clusters. Powders of flowers and leaves have parenchy mafragment, spiral vessels, scalariform vessels, boder pitted vesels, cuticle fragments with stomata, multicellular glandular trichomes. Phytochemical constituents from flora *H. rosa-sinensis* are flavonoids, mucilage, tannins and reducing compounds aqueous extract of flora *H.rosa-sinensis* inhibited 22,93% of alpha-glucosidase enzyme at the concentration of 0,5 mg/ml and 63,43% at the concentration of 1,75 mg/ml, IC_{50} = 1,3 mg/ml, the control was acarbose with IC_{50} = 0,221 mg/ml.

Conclusions: The anatomical and medicinal powder characteristics of help to properly identify this specie and distinguish *H.rosa-sinensis* from other medicinal herbs of the Malvaceae family. The aqueous extract of flora *H.rosa-sinensis* has groups of compounds such as flavonoids, mucilages, tannins and reducing compounds… The concentration of 50% inhibition of alpha-glucosidase activity of the extract was 1,3 mg/ml, equal to 1/6 of that of acarbose 0,221 mg/ml. This study opens up the potential application of flora *H.rosa-sinensis* in the preparation of pharmaceuticals to support the treatment of diabetes.

<PP-52>

The bioactivities of total extract and fractions from *Codonopsis javanica* (blume) root

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Keyword: *Codonopsis javanica* (Blume), antioxidant activity, anti-hyperglycemia activity, anti-inflammation activity, anti-hyperlipidemia, locomotor support activity

Background: *Codonopsis javanica* (Blume) Campanulaceae, also known as the ginseng of the poor, is a precious medicinal herb commonly used in traditional medicine to treat several debilitating diseases and enhance body health. However, the studies about *Codonopsis javanica* bioactivities have remained limited. Therefore, the purpose of this study is to determine the bioactivity such as antioxidant, anti-inflammation, anti-hyperglycemic, anti-hyperlipidemia, and the locomotor activities of *Codonopsis javanica* (Blume).

Methods: In this study, First, *Codonopsis javanica* (Blume) fractions has been extracted. Susequently, their bioactivities were tested *in vitro* and *in vivo*. The antioxidant activity of *Codonopsis javanica* (Blume) was tested by using the total antioxidant activity (TAC), the hydroxyl radical scavenging, and DPPH assays. In order to investigate the motor support ability we performed locomotor assay using IR Actimeter and Rotarod. Furthermore, the antihyperglycemia activity of *Codonopsis javanica* (Blume) was demonstrated on the Alloxan-induced hyperglycemic mice model. The effect of *Codonopsis javanica* (Blume) on Cholesterol and Triglyceride level were conducted on Poloxamer-induced hyperlipidemia mice model. Finally, the anti-inflammatory property of *Codonopsis javanica* (Blume) were tested in Caragennan-induced paw edema in mice.

Results: The results showed that the antioxidant effect of *Codonopsis javanica* (Blume) is moderate. Treatment with *Codonopsis javanica* (Blume) has no toxicity and could increase the level of flexible movement and balance in mice. In addition, *Codonopsis javanica* (Blume) treatment reduced inflammation and edema in the Carageenan-induced paw edema mice model; decreased blood glucose in Alloxan-induced diabetic mice. Eventually, we found that the hyperlipidemic effects of Poloxamer could be attenuated by *C. javanica* root extracts.

Conclusions: These findings suggested that the *C. javanica* root extracts possess many biological activities such as antioxidant, anti-inflammation, anti-hyperglycemia activity, anti-hyperlipidemia, and locomotor support activities. Among all fractions, F2 (ethyl acetate) and F3 (n-butanol) might be the potential fractions.