BOOK OF ABSTRACT

International Conference

on Organic and Applied Chemistry

2022

"Advance Perspective on Organic Chemistry"

14-15th October 2022

ORGANIZED BY DEPARTMENT OF CHEMISTRY
FACULTY OF MATHEMATICS AND NATURAL SCIENCES
UNIVERSITAS BRAWIJAYA

Department of Chemistry, Faculty of Mathematics and Natural Sciences, Brawijaya University
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Opening Speech Dean of Faculty of Science Brawijaya University

Assalamualaikum wr. wb.

On behalf of organizing committee of ICOAC 2022, I would like to extend my warmest welcome to all delegates of ICOAC 2022. Welcome to Malang, one of the educational cities in Indonesia, and welcome to Brawijaya University, Faculty of Mathematics and Sciences, Department of Chemistry. Brawijaya University is the largest university in Malang. Brawijaya University is also included in the top ten best universities in Indonesia. This year, Brawijaya University ranks third, behind UI and UGM, in Webometrics rank.

International Conference on Organic and Applied Chemistry or ICOAC is an annual scientific meeting organized by Organic Chemistry Laboratory, Chemistry Departement, Faculty Mathematics and Sciences. The conference will facilitate researchers and academic members from universities, government institutions, and non-government organization to share their knowledge through the discussion on plenary session, and parallel session of oral presentation.

This year the topic of ICOAC 2022 is "Advance Perspective on Organic Chemistry." I believe that ICOAC 2022 should bring advantages for all participants. They will learn many new aspects of research in the related topics, either from keynote speakers or general participants. In addition, collaborations between Brawijaya University and other universities both from Indonesia and overseas can be initiated.

Finally, I would like to express my gratitude to keynote and invited speakers of ICOAC 2022, for their expertise and knowledge they will bring to the conference, and of course the warm discussion of their talks. Special thanks are also extended to the members of organizing committee for their hard work in bringing this conference together. And last but not least, I would like to thank all of the conference participants who will contribute to making the most memorable ICOAC 2022.

I will also officially open ICOAC 2022, Please enjoy ICOAC 2022 and have a delightful seminar.

Wassalamulaikum wr. wb.

Sincerely yours
Dean of Faculty of Science-Brawijaya University

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About the Symposium

The symposium is aimed to promote mutual exchange between scientists and experts across the nations to disseminate their research findings, discuss innovative ideas to tackle the contemporary problems, and encourage their collaboration. The symposium is organized with the collaboration between Brawijaya University and Okayama University, Ritsumeikan University, Nagoya City University, National Sun Yat-sen University, National University of Singapore, and CNR SCITEC. The meeting is expected to provide an opportunity for young scientists to communicate with the senior scientists, and widen their perspective through discussion with their peers across the nation borders.

Date and Venue

Date : October 14-15th, 2022

Venue : MIPA Center, Faculty of Mathematic and Natural Science

Zoom

Meeting ID : 932 6256 8340

Passcode : icoac2022

URL :

https://univ-brawijaya.zoom.us/j/93778597131?pwd=b3FlUEVuaGV0Q0FXRTkvODNtNC9GZz09

List of Keynote Speakers

Prof. Toru Amaya
Nagoya City University
Japan

Prof. Hideki Okamoto
Okayama University
Japan

Prof. Chun-Hu Chen
National Sun Yat-sen University
Taiwan

Prof. Nicoletta Ravasio
CNR SCITEC
Italy

Prof. Rowan D. Young
National University of Singapore
Singapore

Prof. Silvester Tursiloadi
BRIN, Indonesia

Dr. Sri Fatmawati
ITS, Indonesia

List of Invited Speakers

Dr. Saki Shirako
Ritsumeikan University
Japan

Dr. Elvina Dhiaul Iftitah
Brawijaya University
Indonesia

Dr. Rurini Retnowati
Brawijaya University
Indonesia

Masruri, Ph.D
Brawijaya University
Indonesia

CONFERENCE PROGRAM

FRIDAY, OCT 14th, 2022

Time UTC+7	PROGRAM (OCT 14th, 2022)	
07.30 – 08.00	Registration	Committee
08.00 – 08.05	Opening remarks	*MC:* **Tsaniya Yemima P.**
08.05 – 08.10	Welcome speech by Chairperson	**Siti Mariyah Ulfa, Dr.Sc**
08.10 – 08.20	Welcome speech by Dean of Faculty of Science	**Prof. Dr. Ir. M. Sasmito Djati, MS., IPU, ASEAN Eng**
	Plenary – 1st session	
08.20 – 08.55	**Prof. Toru AMAYA** **(JST: 10.20 – 10.55)** *"Organic Synthesis of Geometrically Unique π-Conjugated Molecules"*	*Moderator:* **Anna Safitri, S.Si., M.Sc., Ph.D**
08.55 – 09.30	**Prof. Chun-Hu Chen** (**Taipe: 09.55 – 10.30**) *"Deposition of Cobalt Manganese Oxides for Electrocatalytic Oxygen Evolution"*	
09.30 – 09.35	*Session break*	
09.35 – 10.10	**Prof. Rowan D. Young** **(SGT: 10.40 – 11.15)** *"A Frustrated Lewis Pair Solution to a Frustrating Problem: Mono-Selective Functionalization of C–F Bonds in Di- and Trifluoromethyl Groups "*	*Moderator:* **Zubaidah Ningsih, Ph.D**
10.10 – 10.45	**Prof. Silvester Tursiloadi** *"Preparation of Sulfated Titania Aerogel Catalyst for Synthesis of Dimer Eugenol as Anti Inflammatory Drugs"*	
10.45– 13.00	Lunch Break	
	Plenary – 2nd session	
13.00 – 13.35	**Dr. Sri Fatmawati** *"Jamu: Indonesian Traditional Medicines in Modern Perspective"*	*Moderator:* **Dr. Akhmad Sabarudin**

Time UTC+7	PROGRAM (OCT 14th, 2022)	
13.35 – 14.10	**Prof. Hideki Okamoto** **(JST:15.35 – 16.10)** " *Photochemical Synthesis of Phenacenes and Their Application to Organic Electronics* "	
14.10 – 14.45	**Prof. Nicoletta Ravasio** (**CEST: 09.10 – 09.45 AM)** *"Chemical Solutions for Agrifood Waste Upcycling"*	
14.45 – 15.00	**Session Break**	
15.00 – 17.00	**Parallel session**	
17.00 – 17.05	**Closing statement – Main Room**	

PARALLEL PROGRAM

FRIDAY, OCT 14th, 2022

Time UTC+7	PROGRAM (OCT 14th, 2022)	
	Parallel Session – Room 1 (Hybrid) **Topic: NAT, SYN, ENE, MMD**	
15.00 – 15.25	**Invited Speaker** **Dr. Elvina Dhiaul Iftitah** Microwave Induced Catalysis for Transforming Eugenol to Vanillin under CoO/$ZnAl_2O_4$ Catalyst	*Moderator:* **Ellya Indahyanti, M.Eng**
15.25 – 15.35	**NAT/O-003** Siti Mariyah Ulfa*[1], Andrian Sucahyo[1], Nur Fitriana[2], Widodo[2], Muhaimin Rifa'I[2], Masruri[1] Cytotoxicity of ethyl acetate sub-fraction of *Curcuma xanthorrhiza* and *Curcuma zedoaria* (Berg.) Roscoe) toward T47D breast cancer cell	
15.35 – 15.45	**NAT/O-004**	

Time UTC+7	PROGRAM (OCT 14th, 2022)	
	Andrian Sucahyo[1], Siti Mariyah Ulfa*[1,2], Dinia Rizqi Dwijayanti[3], Widodo[3], Nishizawa Mikio[4] Flavanones from Ethyl Acetate Fraction of *Caesalpinia sappan* heartwood as Anti-inflammatory and Antioxidant: Isolation, in-vitro, and in-silico approach	
15.45 – 15.55	**NAT/O-005** Tsaniya Shaquilla Y. P.[1], Zubaidah Ningsih[1], Hideki Okamoto[2], Siti Mariyah Ulfa*[1,3] Photophysical Analysis of Naturally Occurring Coumarins Isolated from The Hydrophobic Phase of *Calophyllum inophyllum* Leaves	
15.55 – 16.10	**Discussion**	
16.10 – 16.20	**SYN/O-001** Dwika Putri Pangesti [1], Warsito Warsito [1]*, Masruri Masruri [1] Synthesis Of Eugenol Esters Derivatives As Breast Cancer Drugs	*Moderator:* **Ellya Indahyanti, M.Eng**
16.20 – 16.30	**ENE/O-002** Ahmad Sholeh Romdlon[1], Yuka Fadana[1], Septian Marno[2], Siti Mariyah Ulfa*[1, 3] The production of bioethanol from ethylene glycol as renewable energy using Ni-Cu Based Catalyst	
16.30 – 16.40	**MMD/O-003** A. Ghanaim Fasya[1,2], Warsito[3]*, Elvina Dhiaul Iftitah[3], Rollando[4] Molecular Docking of Selected Volatile Active Compounds From *Hydrilla verticillata* on MMP-2 AND MMP-9 Breast Cancer Proteins	
16.40 – 16.55	**Discussion**	
	Parallel Session – Room 2 (Online) **Topic: NAT, SYN**	
15.00 – 15.25	**Invited Speaker**	*Moderator:*

Time UTC+7	PROGRAM (OCT 14th, 2022)	
	Dr. Saki Shirako (JST: 17.00 – 17.25) Effect of oral administration of pyroglutamyl-leucine, found in Japanese traditional fermented foods	**Dr. Feri Eko Hermanto, M.Si.**
15.25 – 15.35	**NAT/O-001** Listiana Oktavia*[1][2], Dewi Wulandari[1], Wichan Eiadthong[3] , Ahmad Randy[1], Toshiyuki Takano[4], Hiroshi Kamitakahara[4] and Andria Agusta[1],[5] Chemical constituents and biological properties of the root extracts from Prismatomeris plants that are widely distributed in the Southeast Asia region	
15.35 – 15.45	**NAT/O-002** Muhammad Hilmi Afthoni [1], Eva Monica[1], Rollando Rollando[1] Cytotoxic Activity of Flavonoid Compound from Endophytic Fungus Athelia Rolfsii Isolated from *Sterculia quadrifida* R.Br Roo	
15.45 – 15.55	**NAT/O-006** Indra Lasmana Tarigan[1], Nindita Clourisa Amaris Susanto[2], Sutrisno[3], Madyawati Latief*[4] Preliminary Antioxidant and a-glucosidase activity of *P. cannecsens* jack Extract as Functional Food for Antidiabetic Candidate	
15.55 – 16.10	**Discussion**	
16.10 – 16.20	**SYN/O-002** Khoirun Nisyak*[1], A'yunil Hisbiyah[1], Desi Phingkarsa[1] Synthesis of Acetamide Compounds from a-Pinene through Sonochemical Ritter Reaction With Ni/Natural Zeolite Catalyst	*Moderator:* **Dr. Feri Eko Hermanto, M.Si.**
16.20 – 16.30	**SYN/O-003**	

Time UTC+7	PROGRAM (OCT 14th, 2022)	
	Emmy Yuanita *[1], Nurul Hidayah [1], Muhammad Rizal Umami [1], Baiq Nila Sari Ningsih [1], Maria Ulfa [1], Sudirman [1], Ni Komang Tri Dharmayani [1]* Simply Synthesis And Characterization Of Sulfonate Ester Substituted Hydroxyxanthone	
16.30 – 16.40	**SYN/O-004** Andriani Furoida*[1], Osamu Tsutsumi [1] Polymorphism and Mechanochromism Behavior of AIE-active Gold(I) Complex	
16.40 – 16.50	**SYN/O-005** Zidni Akbarorrizki[1], Indah Nur Pramesti*[1] and Mokhamat Ariefin[2] Green Synthesis of Chalcones Derivatives Using $FeCl_3.6H_2O$ as A Catalyst Under Solvent-Free Conditions	
16.50 – 17.10	**Discussion**	
	Parallel Session – Room 3 (online) **Topic: MMD**	
15.00 – 15.25	**Invited Speaker** **Dr. Rurini Retnowati** The Potency of Natural Coloring Extract for Green Identification Methods of Animal Fat Through UV-vis Spectrophotometry	*Moderator:* **M. Hermawan, S.Si**
15.25 – 15.35	**MMD/O-001** Rizki Rachmad Saputra*[1], Siti Mariyah Ulfa*[2], M. Farid Rahman[2], Hideki Okamoto[3] Novel Bromoalkyl-1,4-Benzoquinones as Anti-Inflammatory Candidate Toward COX Signaling: Synthesis, Octanol-Water Solubility, and In Silico Drug-Target Profiling	
15.35 – 15.45	**MMD/O-002** Mokhamat Ariefin*[1], Rizki Rachmad Saputra[1], Indah Nur Pramesti[3]	

Time UTC+7	PROGRAM (OCT 14th, 2022)	
	In Silico Study of Natural Compound on Indonesia Traditional Medicine as A COVID-19 Therapeutic Agent	
15.45 – 15.55	**MMD/O-004** Agus Susilo1,*, Miftakhul Cahyati2, Nurjannah3, Dodyk Pranowo4, Feri Eko Hermanto5,6, Elma Putri Primandasari1 Computer-Aided Investigation of Antiviral Properties of Propolis-Derived Chrysin against Indonesian Serotype of Foot-and-Mouth-Disease Virus	
15.55 – 16.05	**MMD/O-005** Virtual Screening of Antiviral Properties of Bioactive Compounds from Liquid Smoke against 2A Protease of Coxsackievirus-A16 Miftakhul Cahyati[1]*, Agus Susilo[2], Nurjannah[3], Dodyk Pranowo[4], Feri Eko Hermanto[5,6], Elma Putri Primandasari[1]	
16.05 – 16.25	**Discussion**	
	Parallel Session – Room 4 (online) **Topic: ENE**	
15.00 – 15.25	**Invited Speaker** **Masruri, Ph.D**	*Moderator:* **Ade Dirga Rahakbauw, S.Si**
15.25 – 15.35	**ENE/O-001** Gagus Ketut Sunnardianto Reversibility property of nanographene single vacancy for hydrogen storage application	
15.35 – 15.45	**ENE/O-003** Putu Doddy Sutrisna*[1], Juan Anthony Prayogo[1], Andreas Wisnu Warsito[1] The potential of ZIF-7-based mixed matrix membranes for biogas purification	
15.45 – 15.55	**Discussion**	

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ABSTRACT: KEYNOTE LECTURE

Organic Synthesis of Geometrically Unique π-Conjugated Molecules

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The synthesis of geometrically unique π-conjugated molecules has attracted the interest of organic chemists and stimulated their enthusiasm for exploring their functions. Here, I would like to present our recent results on the synthesis and properties of geometrically unique π-conjugated molecules constructed by spirobifluorene linkages.

Bending *p*-oligophenyl compounds with normally linear structures is not always easy, even in modern organic chemistry. In particular, bending *p*-oligophenyl compounds in opposite directions like an S-shape is difficult and challenging. Recently, we have succeeded in the synthesis of such S-shaped *p*-oligophenyl molecules based on a synthetic strategy by the spirobifluorene linkage [1]. In this molecule, two S-shaped *p*-oligophenyl chains support each other.

Furthermore, by linking chiral spirobifluorenes cyclically, we have also achieved a structure that represents a textile patterned unit composed of *p*-quaterphenyls [2]. Although such a textile pattern motif molecule composed of *p*-oligophenyls has never been reported before. We also found that these molecules exhibit an unprecedented type of spiroconjugation. Specifically, DFT calculations revealed that the orbital splitting originating from the spiro-conjugation is clearly affected by the number of chromophores in the quaterphenyl unit.

References

[1] Oniki, J.; Moriuchi, T.; Kamochi, K.; Tobisu, M.; Amaya, T.* *J. Am. Chem. Soc.* 2019, *141*, 18238.
[2] Zhu, K.; Kamochi, K.; Kodama, T.; Tobisu, M.; Amaya T.* *Chem. Sci.* 2020, *11* , 9604.

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Deposition of Cobalt Manganese Oxides for Electrocatalytic Oxygen Evolution

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In this presentation a redox-assisted approach will be demonstrated to produce binary cobalt manganese oxide electrocatalysts with high elemental homogeneity, improved conductivities, and durable stability. This talk will cover nanostructured particles and thin films of cobalt manganese oxides in applications of oxygen evolution reaction with over potentials as low as 0.30 V. The nanostructures in the cobalt manganese oxides can be controlled by varied reaction temperatures, strongly related to the hydrogen peroxide sensing performance. Highly continuous thin films can be deposited with ultrathin thickness (less than 10 nm) over large area (10 x 10 cm2) with simple manners. The thin films demonstrate a strong adhesion on arbitrary substrates comprised of plastics, metals, ceramics, and woods with complex surface textures. Complex oxide deposition can be successfully done to obtain novel thin film electrocatalysts. The film structures, redox reaction principle, and growth control mechanism will be also discussed. This redox approach represents an unprecedented, generic protocol in creating new multi-metal oxide electrocatalysts on diverse electrode surfaces. The water splitting efficiency with anion exchange membrane (AEM) devices has reached as high as 74%.

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A Frustrated Lewis Pair Solution to a Frustrating Problem: Mono-Selective Functionalization of C–F Bonds in Di- and Trifluoromethyl Groups

Rowan D. Young
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Polyfluoromethyl groups generally suffer from 'over-reaction', where multiple C-F bonds are uncontrollably functionalized.[1] To solve this problem, we have developed Frustrated Lewis Pair (FLP) mediated C-F bond activation that allows selective monodefluorination via base capture of intermediate fluorocarbocations.[2] FLP mediated C-F bond activation can be applied to aromatic, heteroaromatic and non-aromatic difluoro and trifluoromethyl groups to generate selectively fluoride substituted phosphonium and pyridinium salts. These salts can be further functionalized via Wittig coupling, nucleophilic substitution, photoredox alkylation, nucleophilic transfer and hydrogenation reactions (*inter alia*) to install a range of functional groups into the activated C-F position.

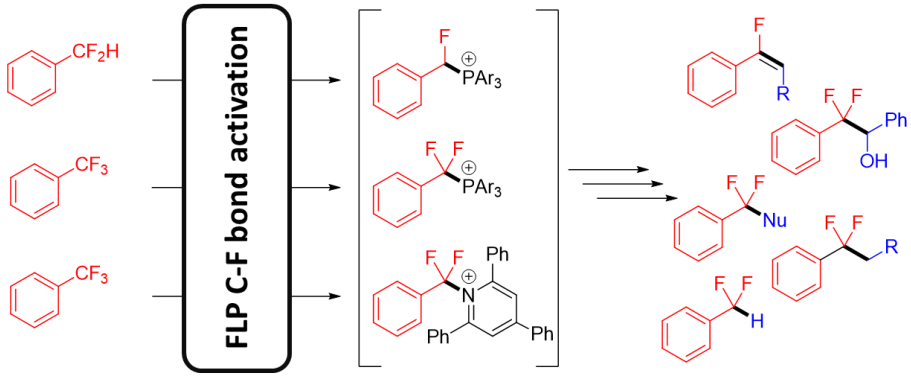

Figure 1. Selective activation and functionalization of difluoromethyl and trifluoromethyl groups mediated by frustrated Lewis pairs (FLPs).

References

1. O'Hagan, D. *Chem. Soc. Rev.*, 2008, 37, 308.
2. (a) Mandal, D.; Gupta, R.; Young, R. D. *J. Am. Chem. Soc.*, 2018, *140*, 10682; (b) Mandal, D.; Gupta, R.; Jaiswal, A. K. ; Young, R. D. *J. Am. Chem. Soc.*, 2020, *142*, 2572.

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Preparation of Sulfated Titania Aerogel Catalyst for Synthesis of Dimer Eugenol as Anti Inflammatory Drugs

Silvester Tursiloadi

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The microstructure of mesoporous sulfated titania aerogel prepared by one-step CO2 supercritical extraction and its catalytic activity has been discussed. Sulfated titania (TiO2-SO42-) aerogel has been prepared through one-step synthesis by the sol-gel method using sulfuric acid as catalyst followed by the one-step CO2 supercritical extraction. Highly porous aerogel with a large surface area (469m2/g) and high porosity (pore volume 1.6cm3/g) has been obtained. Thermal evolution of the gels were evaluated by TGA-DTA, N2 adsorption, TEM and XRD, and the IR absorption spectra measurements were made to discuss the structure of sulfated titania. The bridged bidentate, Ti2SO4 is formed through the sol-gel reaction using sulfuric acid as catalyst and it is stable at temperatures up to 700oC. Due to the presence of surface sulfate, the grain growth of anatase and the phase transformation from anatase to rutile are restrained. The anatase phase is stable after calcination at temperatures up to 700oC, and the specific surface area, total pore volume and average pore diameter of anatase phase do not change significantly after calcination at 600oC. Thermally stable and highly acidic sulfated titania aerogel is attractive as catalyst. The catalytic activity of the sulfated anatase shows good ability for application as a catalyst for synthesis of dimer eugenol. Dimerization of eugeunol reaction with result of Dimer Eugenol crystal, with rendement 10 % (w/w). Dimmer eugenol resulted show better inflammatory activity than parent eugenol and commercial inflammatory drug.

Keywords: sulfated titania aerogel, one-step CO_2 supercritical extraction, dimer eugenol, inflammatory drug.

Jamu: Indonesian Traditional Medicines in Modern Perspective

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Indonesia is among countries having mega-biodiversity in the world and provide a prolific source of medicinal plants for therapeutic agents. Indonesian herbal medicine, so-called Jamu, is formulated based on traditional knowledge of local community for prevention and treatment of various diseases. On the other side, there has been a significant rise on demand of phytopharmaca for global need. These give an opportunity and challenge for us at the same time as evidence-based medicine is required to standardize and support ethnobotanical use. Research on bioactivities of various medicinal plants used in Indonesian herbal remedies has been widely studied, such as antioxidants, antidiabetic, antibacterial, and antifungal and thus becomes our main focus in the Laboratory of Natural Product and Synthetic Chemistry at Department of Chemistry – ITS, which include medicinal plants from genus *Garcinia*, *Curcuma, Phyllantus, Ganoderma* and others. Our extensive projects studying the biological properties and chemical constituents of those plants revealed that they are useful in increasing immunity, preventing several diseases, and increasing stamina, which give us an insight for further development.

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Photochemical Synthesis of Phenacenes and Their Application to Organic Electronics

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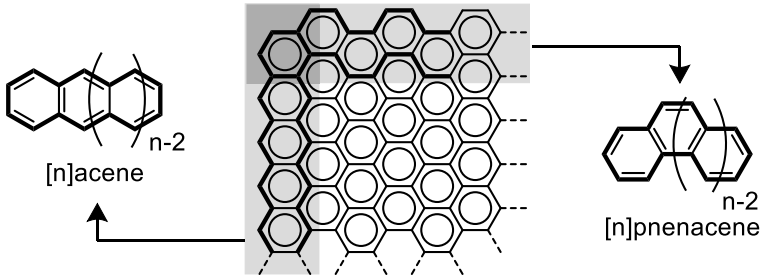
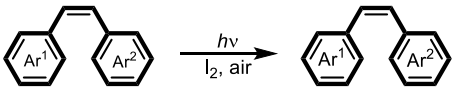
Aromatic molecules with extended π conjugation attract much attention due to their unique chemical and physical properties as well as potential applications to various functional materials namely in organic electronics fields. Acenes, possessing the linearly fused array of benzene rings, have been extensively investigated as aromatic functional materials. Phenacene is another structural category of polycyclic aromatic hydrocarbons with a zigzag-fused benzene array. They are referred as one-dimensional graphene ribbon with the armchair-edge structure. Although phenacenes had been recognized as contents in residue of petroleum industry, they were not applied as functional materials. We have unexpectedly found that phenacenes were promising materials for active layers of organic field effect transistors (FETs) and even for aromatic superconductors. It has been established that phenacene frameworks can be synthesized by Mallory photoreaction. We have fully taken advantages of the Mallory photoreaction and synthesized various phanacenes and their derivatives. It was revealed that the phenacenes were applicable to active layer of FET devices. In this presentation, photochemical synthesis and electronic features of a variety of phenacenes, and their application to organic electronics, such as OFET, will be presented.



General strucurures of acenes and phenacenes



Mallory photoreaction for phenaene synthesisi

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Chemical Solutions for Agrifood Waste Upcycling

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The food supply chain generates enormous amount of waste: veggies residues left over in the fields, side stream of food production, post consumer waste. Most of them are used as feed or in bioenergy production, some are disposed off as waste.

However a green chemistry approach can allow one, once identified the different chemical classes present in the waste, to design specific valorization pathways for each of them also outside the food value chain. Two examples will be reported and discussed: the valorization of rice waste carried out in the frame of RiceRes project and the upcycling of silverskin, a waste of coffee roasting, in the CirCo project.

The multivalorization of rice waste led to green building materials, innovative polymer matrix composites, sterolesters for nutraceutical use and high added value protein hydrolysates[1]. Both chemical and enzymatic processes were used for the upgrade of cellulose, lignin, the oil and the protein fraction of straw, husk and bran.

Extraction of silverskin with supercritical CO_2 led to a fat of unusual composition that was found to be suitable for the formulation of make up products[2]. The subsequent extraction of a powerful antioxidant and its esterification by heterogeneous catalysis led to a product with increased antioxidant properties. Finally the residue was used as a replacement of virgin cellulose in the production of graphic paper. A detailed LCA analysis allowed to state that substitution of 15% virgin cellulose with silverskin derived cellulose can reduce the environmental impact of paper production by 10% and greenhouse gas (GHG) emissions by 13% compared to conventional production[3].

The hydrogenation of lactose, the main component of cheese whey, to sorbitol and dulcitol will also be discussed[4].

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2. R. Nasti, A. Galeazzi, S. Marzorati, F. Zaccheria, N. Ravasio, G.L.Bozzano, F. Manenti, L. Verotta, Waste and Biomass Valorization, 2021, 12, 6021-6033
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ABSTRACT: INVITED SPEAKERS

INTERNATIONAL CONFERENCE ON ORGANIC AND APPLIED CHEMISTRY (ICOAC) 2022
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Effect of oral administration of pyroglutamyl-leucine, found in Japanese traditional fermented foods

Saki Shirako

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Food proteins are digested by protease to produce food peptides. Also it has been shown that some peptides in foods are modified during processing and storage. Pyroglutamyl-leucine (pyroGlu-Leu, pEL), a di-peptide, is one of the example of food-derived peptides. It is widely present in wheat gluten hydrolysates and Japanese traditional fermented foods, such as soy paste (miso), soy sauce (shoyu), and Japanese rice wine (sake). It has been shown that treatment of pyroGlu-Leu has some beneficial effect, such as anti-inflammation, hepato-protective effect, attenuation of DSS-induced colitis and dysbiosis, and so on.

In ICOAC, I will introduce one of our study; Attenuation of high-fat diet induced dysbiosis by pyroGlu-Leu. In this study, we used rats divided into four groups, fed normal or high fat diet, received vehicle or 1.0 mg/kg body weight of pyroGlu-Leu. Micorbiota was evaluated by quantification of Firmicutes and Bacteroidetes in rats' feces by using qPCR. To elucidate the mechanism of how small dose of pyroGlu-Leu attenuated dysbiosis, we evaluated antimicrobial peptides which is secreted from ileum as host defense system by LC-MS.

As a result, we found that administration of pyroGlu-Leu attenuated high fat diet-induced dysbiosis. Moreover, pyroGlu-Leu increased propeptide form of antimicrobial peptide in ileum and active form of it in lumen. These results suggest that oral administration of pyroGlu-Leu attenuates dysbiosis in colon by increasing secretion of host antiimicrobial peptide in ileum.

Effect of oral administration of pyroglutamyl-leucine, found in Japanese traditional fermented foods

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Microwave induced catalysis process based on $CoO/ZnAl_2O_4$ catalysts, was reported for the two-step transforming eugenol to vanillin. Effects of catalyst load and irradiation time for the efficiency of catalytic oxidation were studied. The products of two step transforming were studied by FTIR and GCMS. Results indicated that interaction between microwave irradiation and $CoO/ZnAl_2O_4$ catalyst showed much higher catalytic oxidation activity than under reflux heating. Significantly, transforming eugenol to vanillin efficiency reached 67.79 % under optimal conditions with microwave power of 400 W, 4% catalyst and reaction time of 15 min. Comparison with one pot catalytic oxidation under reflux heating method using ZnO, CoO, dan $ZnAl_2O_4$ catalysts also reported.

Keywords: eugenol, vanillin, microwave-induced catalysis, $CoO/ZnAl_2O4$ catalyst

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The Potency of Natural Coloring Extract for Green Identification Methods of Animal Fat Through UV-vis Spectrophotometry

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Environmental concerns are becoming more widespread. Chemistry must follow the trend of sustainable development and be "green" or "clean." Thus, the "Twelve Principles of Green Chemistry" guidelines mostly addressed the facets of synthetic chemistry, but they also included the foundation of green chemistry. Green Chemistry is defined as the exploitation of techniques and methodologies aiming to reduce or eliminate the use of chemicals that are hazardous to human health or the environment and thus the amounts and toxicity of waste. One method in the development of affordable and ecologically friendly green identification is the use of natural coloring reagents from plant extracts for chemical analysis. As an alternative to the carcinogenic diazonium reagent, this work seeks to identify animal fats by UV-vis spectrophotometric technique utilizing natural coloring reagents of several extracts. The basis for the diazonium reagent test is that red dye is composed of hydrophobic molecules. In comparison to plant extracts having polar main compounds, extracts containing non-polar major compounds produced good results in the identification of fats. Although the UV-Vis spectrum profiles of the animal fats with and without the addition of extract reagents showed various UV-vis spectrum profiles, the profiles obtained were different. Based on the finding, it can be said that utilizing ethylacetate as a solvent, together with a combination of natural coloring extracts, and UV-Vis spectrophotometry method can be used to distinguish between each type of animal fat.

SYMPOSIUM

Organic Synthesis (SYN)

SYN/O-001

Synthesis Of Eugenol Esters Derivatives As Breast Cancer Drugs

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ABSTRACT

Breast cancer is the commonest cause of cancer death in women worldwide due to the high-risk cardiotoxicity and cytotoxicity treatments. So the attention to scientific and commercial cancer treatment leads to anticancer drugs made from natural ingredients because they are considered effective drugs but have low cytotoxic effects. The Discovery of natural compounds such as eugenol from clove essential oil has shown anticancer ability. Interestingly, the modification of the structure of the eugenol ester derivative compound combined with other essential-oil compounds has a better ability as an anticancer. The screening in-silico studies were used to see the effectiveness and efficiency of the compounds as breast cancer drug candidates by comparing with the doxorubicin cancer drug standard, 18 eugenol ester derivatives docked against five cancer proteins as representatives of breast cancer such as MMP9, MMP2, Cyclin A2 (CCNA2), BAK, and P53. The best compounds for screening will be synthesized with steglich esterification using DCC and DMAP catalysts. The in-silico screening result showed eugenol salicylate and isoeugenol salicylate have the best binding affinity values of -8.5 and -8.9 kcal/ mol in MMP9. The synthesis result of eugenol salicylate and isoeugenol salicylate shows the Rf value of TLC with eluent n-hexane: ethyl acetate (9:1) is 0.58, whereas LCMS results for each compound showed yield values of 48% (RT: 10.79) and 60% (RT: 9.67).

SYN/O-002

Synthesis of Acetamide Compounds from α-Pinene through Sonochemical Ritter Reaction With Ni/Natural Zeolite Catalyst

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ABSTRACT

α-pinene is the main compound of turpentine oil that can be derivatized as drug candidate compounds. α-pinene was derivatized through the Ritter reaction with ultrasonication into amide compounds. Starting materials used are α-pinene and acetonitrile. The ultrasonication Ritter reaction method was carried out using a variety of catalysts, namely activated natural zeolite (ZAA), Ni/ZAA, and sulfuric acid. The Ni/ZAA catalyst was made by impregnating Ni (15%) metal on activated natural zeolite. The catalyst used was characterized by crystallinity by XRD and morphology by SEM-EDX. The XRD spectra of the Ni/ZAA catalyst showed Ni peaks at 2θ = 43.224º and 62.7864º. The resulting reaction products were analyzed for functional groups by FT-IR and the spectrum of the compounds using KG-SM. Based on the results, the acetamide compound was obtained on a Ni/ZAA catalyst with a yield of 3.86%, with the α-pinene conversion being 54.56%. The acidity of the catalyst used influences these results, and acidity affects the formation of carbocations from α-pinene.

SYN/O-003

SIMPLY SYNTHESIS AND CHARACTERIZATION OF SULFONATE ESTER SUBSTITUTED HYDROXYXANTHONE

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ABSTRACT

The synthesis of hydroxyxanthone (1,3 dihydroxyxanthone (DHX) and 1,3,7 trihydroxyxanthone (THX) substituted sulfonate ester was successfully carried out. The synthesis started with a cyclization reaction to form a hydroxyxanthone, followed by the formation of a sulfonate compound by chlorosulfonic acid reagent, and ended through an esterification with ethanol. Characterization of compounds using IR and 1H-NMR. The percentage of synthesis of sulfonatester compounds for DHX and THX was 33 % 45 %, respectively.

SYN/O-004

Polymorphism and Mechanochromism Behavior of AIE-active Gold(I) Complex

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ABSTRACT

In the past two decades, the development of aggregation-induced emission (AIE)-active molecules, in which the molecules are non-emissive in dilute solution and strongly emissive in aggregated states is increasingly attractive.[1] The solid-state luminescence of organic materials relies strongly on their molecular packing and intermolecular interaction. In recent years, there has been growing interest in materials that can show distinct solid-state luminescence from one chromophore by taking advantage of polymorphism behavior. Polymorphic materials possess more than one crystalline phase, where each phase shows different emission color. Especially, mechanochromic luminescence has received considerable attention due to its wide potential in sensors, probes, and memory devices. In these systems, mechanical force (e.g., mechanical grinding and stretching) could induce a significant change in optical properties mostly due to the change in molecular arrangements. Gold complex is an attractive material to induce strong luminescence in aggregated states and stimuli-responsive luminescence behavior owing to the unique Au–Au (aurophilic) interaction. Indeed, numerous studies have reported various gold complexes with luminescence color sensitivity toward external stimuli (mechanical force, heat, pressure).[2,3] In this study, We designed and synthesized gold complexes with biphenyl or cyclohexylphenyl and isocyanide ligands. These type of complexes having ligands with less steric bulkiness around Au atoms is favorable to manifest aurophilic interaction. Photophysical behaviors of the gold complexes in various states were discussed based on not only their primary structures but also the structure of molecular aggragates. Both complexes are AIE-active, with strong room-temperature phosphorescence (RTP) in the crystal. Interestingly, CP exhibited intriguing stimuli-responsive luminescence by having both polymorphism and mechanochromism behavior. Distinct emission color was observed in CP complex under different recrystallization conditions. Such emission color-dependent is likely to attribute to the change in the aggregated structure between crystal polymorphs as well as the ground crystal. 1) Ben Zhong Tang et al., J. Mater. Chem., 2001, 11, 2974 2) Hajime Ito et al., Angew. Chem. Int. Ed., 2013, 52, 12828. 3) Kaori Fujisawa et al., Sci Rep., 2015, 5, 7934

SYN/O-005

Green Synthesis of Chalcones Derivatives Using FeCl3.6H2O as A Catalyst Under Solvent-Free Conditions

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ABSTRACT

Chalcone is a precursor of a group of flavonoid and isoflavonoid compounds that are commonly found in plants in Indonesia. Chalcone compounds and their derivatives are reported to have antibacterial, antioxidant, anti-inflammatory, antimalarial, anticancer, antitumor, analgesic, and antipyretic activities. Chalcones can be synthesized through a Claisen-Smidth condensation reaction between aromatic aldehydes and ketones using an acid or base catalyst followed by a dehydration reaction. This study aimed to synthesize chalcone derivatives using eco-friendly non-toxic FeCl3.6H2O catalysts under solvent-free conditions. Our experiment was carried out to synthesize some chalcone derivatives at 100-140 oC by stirring process. In this study, the synthesis of chalcone derivatives was started with 10 mmol of various benzaldehyde (p-hydroxybenzaldehyde; p-methoxybenzaldehyde) and 10 mmol acetophenone in the presence of 0.1 mmol FeCl3.6H2O catalysts then the mixture was stirred for 20, 40 and 60 minutes. The product was then purified by recrystallization using ethanol. The purity of chalcones yielded was investigated by Thin Layer Chromatography (TLC) and melting point test while the structure was then characterized by UV-Vis and GC-MS analysis.

SYMPOSIUM

Chemistry of Natural Products (NAT)

NAT/O-001

Chemical constituents and biological properties of the root extracts from Prismatomeris plants that are widely distributed in the Southeast Asia region

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ABSTRACT

This study aims to reveal the chemical constituent and biological activities of previously unreported Primatomeris beccariana (Pb), natively grown in the Borneo island of Indonesia. Two other Prismatomeris plants, Prismatomeris tetrandra (Pt), and Prismatomeris griffithii (Pg) collected from Thailand were compared chemically as guidance to obtain the chemical information of Pb. Moreover, the biological properties (antimicrobial, antioxidant, and cytotoxicity) of comparison were also established to predict the pharmacologically important substances in the root bark extract of three Primatomeris plants collected from different regions in Southeast Asia. The chemical profiling obtained from HPLC and LCMS data described the domination of the anthraquinones group in the three Prismatomeris plants. As compared to Pt and Pg, the chemical diversity of Pb is identified as rubiadin, rubiadin-1-methyl ether, 3-Hydroxyanthraquinone 2-carbaldehyde, 3-Hydroxyanthraquinone 2-carbaldehyde, 5-hydroxyl-1,2,3,4-tetramethoxy-9,10-anthraquinone, 2-(hydroxymethyl)-5,6-dimethoxy-1,3-dihydroxy-9,10 anthraquinone and C28H50O13 (unidentified). More interestingly, LCMS data revealed the relatively similar chemical constituents in the three Prismtomeris samples except for one compound which was putatively identified as 2-(hydroxymethyl)-5,6-dimethoxy-1,3-dihydroxy-9,10 anthraquinone (C17H14O7), 1,5,6-Trimethoxy-2-methyl-3-hydroxyl-9,10-anthraquinone (C18H16O6) and C12H33N (unidentified) in Pb, Pt and Pg respectively. Consequently, they are potentially developed as a chemotaxonomic agent for the respective Prismatomeris samples. The biological properties described the strong potency as antibacterial agents from methanolic extracts of three Prismatomeris samples against S. aureus bacteria. The Minimum Inhibitory Concentration (MIC) values of methanolic extract varied from 32µg/mL to 62 µg/mL, while the ethyl acetate extract exhibited a relatively modest activity with MIC values of more than 128 µg/mL. Antioxidant activity investigation showed no significant activity against DPPH radical scavenging assay. On the other hand, the cytotoxicity test announced a relatively good potency of ethyl acetate extract of Pb. While the growth of Hep-G2 cell lines was observed to be suppressed proportionally by ethyl acetate extract of Pb and Pt Keywords: anthraquinones, antibacterial, antioxidant, cytotoxicity, LCMS, Primatomeris

NAT/O-002

Cytotoxic Activity of Flavonoid Compound from Endophytic Fungus Athelia Rolfsii Isolated from Sterculia Quadrifida R.Br Roo

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ABSTRACT

A flavonoid compound was obtained from the endophytic fungus Athelia rolfsii which was isolated from the medicinally significant plant, Sterculia quadrifida R.Br root. The chemical structures of a flavonoid were elucidated on the basis of HR-ESI-MS and NMR data including 1H, 13C, and HMQC spectra namely pinostrobin. Cytotoxicity was evaluated against breast cancer cell lines T47D. Pinostrobin showed significant cytotoxicity on T47D cell lines with IC50 value ranged from 3.31 µg/mL.

NAT/O-003

Cytotoxicity of ethyl acetate sub-fraction of Curcuma xanthorrhiza and Curcuma zedoaria (Berg.) Roscoe) toward T47D breast cancer cell

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ABSTRACT

A long history of the uses of herbal medicine in Asia, including Indonesia comes from folklore with limited information about the constituents responsible for the pharmacological effects. Here, we reported the extraction of Curcuma xanthorrhiza (CX) and Curcuma zedoaria (Berg.) Roscoe) (CZ) root using alcohol followed by solvent partition using ethyl acetate and determined the active constituent for anticancer. The partition of CX and CZ crude extract gave 67.93% and 64.3% ethyl acetate fractions, respectively. Cytotoxicity screening of CX and CZ ethyl acetate fraction showed that both curcumas had high toxicity. Purification using SiO2 column chromatography gave 9 subfractions of CX and 11 subfractions of CZ. Bioactivity analysis of each subfraction using the T47D breast cancer cell line showed a prospective result. Subfraction CX-F3 and CX-F4 have the highest toxicity with IC50 54,8 ± 1,5 µg/mL and 59,3 ± 3,0 µg/mL, respectively. For CZ, subfractions CZ-F1, CZ-F2, CZ-F4, CZ-F5, and CZ-F8 have IC50 between 50-60 µg/mL. Based on this result, the constituent in the ethyl acetate fraction of CX and CZ is suggested to have a high potency as an anticancer agent.

NAT/O-004

Flavanones from Ethyl Acetate Fraction of Caesalpinia sappan heartwood as Anti-inflammatory and Antioxidant: Isolation, in-vitro, and in-silico approach

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ABSTRACT

Caesalpinia sappan, commonly known as secang by Indonesian people, has been widely used for its analgesic, antioxidant, anti-diabetes, anti-inflammatory, anti-microbial, and anticancer activities. Flavonoids are reported as the most responsible constituents for that pharmacology effect. Flavanone, one of the flavonoid classes, has a particular interest because it has a wide range of compounds with O-substituents, such as hydroxy, methoxy, and O-glycosyl. In this study, the isolation of constituents in C. sappan was carried out by MeOH, followed by solvent partition using ethyl acetate. Continuing the purification of ethyl acetate fraction with SiO2 column chromatography gave 9 sub-fractions (A1-A9). Analysis of antioxidants suggested that A7, A6, and A5 have the highest antioxidant activities with IC50 values of 0.11 ± 0.02, 0.18 ± 0.03, and 0.19 ± 0.01 ppm, respectively. An anti-inflammatory test was carried out in-vitro using RAW 264.7 cell macrophage to evaluate the suppression of nitric oxide (NO) induced by LPS. Fractions A3, A6, and A7 are giving promising results in the suppression of NO production. Further analysis using LC-MS to these fractions gave poriol and pinostrobin (flavanone derivatives) and hydroxybrazilin consist in fractions A3, A5, A6, and A7. However, brazilin is not detected by this analysis. In-silico analysis by molecular docking revealed that pinostrobin and poriol show a better result to inhibit iNOS, COX-1, COX-2, IL-1β, and TNF-α. The hydroxyl group from poriol and pinostrobrin are responsible for their antioxidant activities, while the methoxy group in pinostrobin can increase its anti-inflammatory activity shown by the better binding affinity. Taken together, the result suggests that the flavanones from C. sappan have potent antioxidant and anti-inflammatory activities that may be useful in preventing various diseases.

NAT/O-005

Photophysical Analysis of Naturally Occurring Coumarins Isolated from The Hydrophobic Phase of Calophyllum inophyllum Leaves

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ABSTRACT

Coumarin moiety from the natural product was rapidly observed because of its photochemical and photophysical properties that show excellent potential as laser dyes and fluorescent probes. Recently, four new coumarins from the leave of Calophyllum inophyllum have been identified. Since structure differences greatly affect the photophysical and photochemical properties, in this research the isolation of coumarin from the leave of C. inophyllum cultivated in Indonesia was carried out. Low polarity solvents, that is hexane and chloroform were used for partitioning crude MeOH extract of C. inophyllum. From 600 g of C. inophyllum dry leave, 18.76% of MeOH extract obtained. Solvent partition using hexane and chloroform gives 5.21% and 0.93%, respectively. Qualitative phytochemical analysis of hexane fraction suggested that coumarin derivatives are collected more in hexane fraction than in chloroform. Further purification of hexane fraction using SiO2 and analysis of isolated compound using LCMS, NMR spectroscopy and spectrofluorometer is conducted to explain the photophysical properties of naturally occurring coumarins from C. inophyllum.

NAT/O-006

Preliminary Antioxidant and α-glucosidase activity of P. cannecsens jack Extract as Functional Food for Antidiabetic Candidate

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ABSTRACT

Diabetes mellitus is a metabolic syndrome disease characterized by a hyperglycemic state due to the pancreas' inability/ not being able to produce enough insulin. The body is unable to use the insulin properly that is producing effectively. Delaying treatment of the disease will cause several complications and even could lead to premature death. One of the antidiabetic alternatives by utilizing medicinal plants as both extracts and functional foods formulated. Generally, functional food is a term for food-driven from bioactive components, which can provide health benefits, beyond the benefits provided by the nutrients contained therein. Based on ethnomedicine, one of the plants that known the potentiality to be developed as an alternative to hypoglycemic functional drinks is the Sungkai (Peronema canescens Jack). P. canescens leaves contain several secondary metabolites that play a role in improving insulin sensitivity by improving sugar metabolism in the body. This study aims to develop a functional tea antioxidant-rich from P. canescens leaves extract as a healthy drink for diabetes. The characterization of bioactive compounds used the DPPH method and Alpha-glucosidase inhibition. Tea was formulated by adding four different extract concentrations, 5%, 10%, 15%, and 20%, respectively, then determined tea organoleptic and antioxidant activity. The results showed that the IC50 value of the antioxidant activity of P. canescens leaves extract in n-hexane and ethyl acetate was inactive, 1023,556 and 884.854 ppm respectively while IC50 value 291,588 ppm for ethanol solvent. Somehow, the inhibitory activity test showed that the 10ppm ethanol extract had 0.079% % inhibition belongs to weak, while the acarbose control was 95%. These results indicate that the ethanol extract of P. canescens leaves was inhibits the α-glucosidase enzyme, IC50 20ppm. The antidiabetic activity was then verified by measured on the blood sugar levels of mice. The test results showed that the highest decrease in blood sugar levels was at PE4 (extract 800mg/kg BW). Our finding in this research is that in functional drinks, the highest decrease in blood sugar levels was at TF2 (10% extract).

SYMPOSIUM

Molecular Modeling in Drug Design (MMD)

MMD/O-001

Novel Bromoalkyl-1,4-Benzoquinones as Anti-Inflammatory Candidate Toward COX Signaling: Synthesis, Octanol-Water Solubility, and In Silico Drug-Target Profiling

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ABSTRACT

The main structure of novel bromoalkyl-1,4-benzoquinones is quinoid ring that can be modified to increase the bioavailability as a drug candidate. In this research, the modifications were carried out as 2-(4-bromobutyl)-3.5-dimethyl-1,4-benzoquinone (C4), 2-(7-bromoheptyl)-3,5-dimethyl-1,4-benzoquinone (C7), and 2-(10-bromodecyl)-3.5-dimethyl-1,4-benzoquinone (C10) by bromoalkylation reaction. Target compounds were successfully synthesized in 74.72%, 11.97%, and 26.67% yield, respectively. Chemical constituents of product were identified by Fourier-transform infrared spectroscopy (FTIR), nuclear magnetic resonance spectroscopy (^{1}H-NMR and ^{13}C-NMR), and liquid chromatography (LC)-MS. Then, synthesized compounds were investigated its properties by in vitro solubility test in octanol-water using HPLC. Solubility test results showed that the products C4, C7, and C10 had greater solubility in octanol phase than in the water phase. According to solubility assay, C4, C7, and C10 showed partition coefficients of 1.6; 4.95; 1.74 and compare to thymoquinone (positive control) partition coefficient was 2.58 at pH 7.4. Potency as drugs of synthesized compounds were evaluated by molecular docking using COX-1 (ID 1EQG) and COX-2 (ID 1CX2) as COX signaling receptor. In silico studies depicted that C7 activity has great binding affinity toward COX-1 and COX-2, respectively. Especially for the activity toward COX-1 receptor, the binding affinity of C7 was equal to Ibuprofen/native ligand (-7.7 kcal mol^{-1}). The C7 has two molecular interactions toward COX-1, one hydrogen bond (Tyr385) and one hydrophobic (Ser530, Leu531, Ala527, Ser353, Ile523, Val349, Phe518, Leu384, Trp387, Phe381, Gly526, Tyr355, Leu359, Arg120, Val116, Tyr348). Otherwise, signaling activity of C7 toward COX-2 receptor in binding affinity showed -7.7 kcal mol^{-1} that slightly lower than SC-558/native ligand -11.3 kcal mol^{-1}. Furthermore, profiling drug-target interaction between C7 and COX-1 receptor was illustrated by binding similarity. The binding similarity of C7 was 66.67%. Additionally, the ADME parameters and Lipinski's rule of five suggested that these compounds would have good drug-likeness. Keyword: Anti-inflammatory, Benzoquinones, Bromoalkylation, in vitro, Partition Coefficient, LogP, in silico, COX signaling, Drug-likeness, ADME, Lipinski's rule of five

In Silico Study of Natural Compound on Indonesia Traditional Medicine as A COVID-19 Therapeutic Agent

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ABSTRACT

In 2019, the coronavirus disease (COVID-19), which started in Wuhan, China, spread throughout the world. COVID-19 is a disease that infects the human respiratory tract. COVID-19 has developed more widely and is reported to have mutated into several variants, one of which is Omicron. Until now, no specific antiviral drug compound used to cure COVID-19. Therefore, several drugs are used to treat COVID-19 (such as antiviral drugs, antibiotics, and interferons) without evidence of human efficacy. However, the use of this drug is limited due to side effects. Therefore, the use of natural products as therapeutic agents found in nature can be explored for the treatment of COVID-19. Formulating various herbs with the ingredient rosella (Hibiscus sabdariffa), sappanwood (Caesalpinia sappan), ginger (Zingiber officinale) and honey is one traditional drink from Indonesia. These ingredients contain a lot of natural products that potent to be drug compounds, such as rosmaric acid (1) (from rosella), brazilin (2) (contained in sappan wood), 10-gingerol (3) (found in ginger), and kaemferol (4) (found in honey) has been explored their potency to be a COVID-19 therapeutic agent. The docking method has been validated by redocking the native ligand to the Mpro of COVID-19 omicron variant (PDB ID: 7TOB) as a receptor protein. Compound (4) (ΔG = -8.2 kcal/mol) has a more negative binding energy than the native ligand (ΔG = -8.1 kcal/mol) of 7TOB. On the other hand, the binding energy of compounds (1), (2), and (3) are -7.6 kcal/mol, -7.4 kcal/mol, and -5.5 kcal/mol. Based on the combined analysis of binding affinity and binding similarity of active sites, the compound in the traditional drinks from Indonesia is expected to be a potential therapeutic agent for COVID-19. Keywords: COVID-19, Omicron, Mpro

MOLECULAR DOCKING OF SELECTED VOLATILE ACTIVE COMPOUNDS FROM Hydrilla verticillata ON MMP-2 AND MMP-9 BREAST CANCER PROTEINS

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ABSTRACT

Hydrilla verticillata is an aquatic plant that contains various volatile active compounds that potential as candidates for breast cancer inhibitors. Several active compounds can inhibit cancer through the mechanism of metastasis and angiogenesis, including by inhibiting Matrix Metalloprotein (MMP) reseptors. The docking of volatile active compounds in Hydrilla verticillata on MMP-2 and MMP-9 proteins has been carried out to determine the binding affinity and type of binding between the ligand and the receptor. Six volatile active compounds Hydrilla verticillata which have the potential to inhibit the growth of breast cancer cells were taken from the PubChem database. Molecular docking of these compounds to MMP-2 and MMP-9 receptors (3AYU and 4H1Q) was carried out using software such as RSCB Protein Data Bank, PyrX Virtual Screening Tool and BIOVIA Discovery Studio Visualizer. The results showed that phytol, 14-methylpentadecanoic acid, 1,2-Benzenedicarboxylic acid butyl octyl ester, cis-10-Octadecenoic acid, trans-10-Octadecenoic acid and Ergost-5-en-3-ol, 22,23-dimethyl-, acetate had binding affinities of -6.3, -6.2, -7.0, -6.4, -5.7 and 8.6 kcal/mol towards 3AYU MMP-2 receptor and -4.5, -5.2, -5.7, -4.1 and 8,5 kcal/mol towards 4H1Q MMP-9 receptor. While the native ligand has a binding affinity of 8.0 and 7.8 kcal/mol. Some volatile active compounds from Hydrylla verticillata have a better binding affinity than native ligand, so it can be concluded that these compounds have the potential as anti-cancer

MMD/O-004

Computer-Aided Investigation of Antiviral Properties of Propolis-Derived Chrysin against Indonesian Serotype of Foot-and-Mouth-Disease Virus

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ABSTRACT

Propolis has been evaluated for broad bioactivities. Among several compounds found in propolis, Chrysin is one of the most abundant constituents in the propolis. Although the antiviral properties of Chrysin against the Foot-and-Mouth-Disease Virus (FMDV) had been reported, the bioactivity against the Indonesian serotype remains unknown. Thus, this study will evaluate the effectivity of Chrysin in inhibiting replication of Indonesian serotype FMDV. First, Density Functional Theory (DFT) was employed to observe the electronegativity of the Chrysin structure before the molecular docking analysis. Besides, the structure of 3C Protease (3CP) was homology-modeled, then docked with Chrysin, and continued to the molecular dynamics analysis. The catalytic residues of 3CP were predicted using the COFACTOR webserver to guide the grid box position for molecular docking analysis. The result showed that Chrysin had a great electronegativity map to perform its interaction against 3CP. Molecular docking also revealed the low energy requirement of Chrysin to bind with the catalytic site of 3CP. The binding of Chrysin also did not affect the structural integrity of 3CP compared to the unbound structure. Chrysin also had excellent stability during the binding to 3CP, along with a stable number of hydrogen bonds and binding energy. In summary, Chrysin has excellent potential to prevent FMDV infection severity through viral replication inhibitions.

MMD/O-005

Virtual Screening of Antiviral Properties of Bioactive Compounds from Liquid Smoke against 2A Protease of Coxsackievirus-A16

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ABSTRACT

Hand, foot, and mouth disease (HFMD) is a contagious disease in toddlers and youth, mainly caused by Coxsackievirus-A16 (CA16) infection. On the other hand, liquid smoke (LS) contains numerous bioactive molecules, which improve the value beyond it's main application as food seasonings. Although the bioactivity of liquid smoke against mouth disease was reported, it's exact mechanism remains inconclusive. Through computational analysis, this research will explore the potential bioactivity of several compounds from LS as an alternative therapeutic agent for HFMD. The investigation started with exploring bioactive compounds for toxicity evaluation using ProTox-II. The passed compounds were then directed for molecular docking against 2A Protease (2AP) of CA16 to predict their antiviral properties. Compound with specific binding against the catalytic site of 2AP and resemble the binding energy of Benzydamine as the main medications of HFMD, then directed for molecular dynamics analysis. As a result, only 21 compounds of LS have fewer toxicity properties. Molecular docking also discovered that Acetosyringone and Homosyringic Acid had lower binding energy than other pre-screened compounds. Those compounds also interacted with HIS21, TYR89, PRO107, and CYS110 as the substrate-binding site of 2AP. Additionally, the binding of those compounds to 2AP showed structural stability from protein atom backbone and ligands structure according to the molecular dynamics simulations. The fluctuations of per-residue were also minimum, and the binding energy remained stable along the simulations. The solvent-accessible surface area (SASA) also displayed a relatively stable conformation at the catalytic cleft position upon binding with the Acetosyringone and Homosyringic Acid compared to Benzydamine. Therefore, the protective effect of LS against HFMD may occur through antiviral activity against CA16 by inhibition of viral replications. Keywords: 2A Protease; Acetosyringone; Coxsackievirus-A16; Hand, Foot, and Mouth Disease; Homosyringic Acid; Liquid Smoke.

SYMPOSIUM

Renewable Energy (ENE)

ENE/O-001

Reversibility property of nanographene single vacancy for hydrogen storage application

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ABSTRACT

We are aiming to find the best structure of nanographene for hydrogen storage application. Although very long research has been conducted for solid-state hydrogen storage application, the efficiency of hydrogen adsorption-desorption process has not yet been finalized. We found a new self-catalyst in nanographene single vacancy to improve the reversibility of hydrogen adsorption-desorption process by combining the effect of edge state and single vacancy in nanographene for optimizing the reversibility process of hydrogen adsorption-desorption.

ENE/O-002

The production of bioethanol from ethylene glycol as renewable energy using Ni-Cu Based Catalyst

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ABSTRACT

Renewable energy is energy sources from natural processes which continuously replenished, and the resources are inexhaustible. The use of renewable energy is promising since it can reduce gas emissions compared to fossil fuels. Biomass is one of the renewable resources since its content with the polymer of carbon, such as cellulose, hemicellulose, and lignin. Catalytic hydrogenation of cellulose resulted in ethylene glycol as an intermediate product. Then, continue this reaction gives ethanol. In this research, catalytic hydrogenation of ethylene glycol was carried out using Ni-Cu-based catalysts. The reaction was conducted in an autoclave batch reactor using 2 MPa H2 gas at 300oC for 2-4 hours. Analysis of the products using gas chromatography gave 29.26% ethanol using the 2%Ni-20%Cu/SiO2 after 4 h of reaction time. The other products detected are aliphatic hydrocarbons, such as 1-propanol, 2-butanone, 1-hydroxyl-2-butanone, and cyclic hydrocarbons such as 1,4-dioxane, and cyclohexane. From this result, it is suggested that the combination of Ni-Cu catalyst is important to promote hydrogenation and/or hydrogenolysis reaction of ethylene glycol into ethanol. Further experiment proposes to increase the ethanol yield and clarify the mechanism of those reactions catalyzed by Ni-Cu. Keywords: hydrogenation, hydrogenolysis, Ni-Cu based catalyst, fossil fuels, biomass

The potential of ZIF-7-based mixed matrix membranes for biogas purification

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ABSTRACT

Gas separation technology using membranes is an important requirement for biogas upgradation process to ensure the alternative energy possesses high calorific value due to low CO2 concentration. However, poor operating stability, mainly at high pressure and plasticization of membranes, are constraints to the use of membranes, especially polymeric membranes. The trade-off constraint where high selectivity will have an impact on membrane permeability can be overcome by using mixed matrix membranes (MMMs) which are made of nanofiller particles in the polymer membrane matrix. In making MMMs, the accurate type and concentration of particles are needed to produce a good membrane. The objective of this research is to synthesis and characterize MMMs from the polymer matrix of cellulose acetate and ZIF-7 particles. ZIF-7 particles are prepared at room temperature by two different methods. The difference in the method is the type of solvent used, namely DMF and ethanol-water mixture. The synthesized membrane was analyzed using SEM-EDX, FTIR, XRD, and DSC. The results of the MMMs morphological analysis using SEM-EDX showed that ZIF-7 particles could be evenly distributed with little agglomeration. The increase in the concentration of ZIF-7 used also showed an increasing trend of agglomeration that occurred in both MMMs. In MMMs cellulose acetate / ZIF-7 DMF solvent, an increase in the concentration of ZIF-7 showed an additional peak and a decrease in %transmittance with FTIR analysis which indicated the stronger the bond between ZIF-7 particles and cellulose acetate polymer, whereas in MMMs cellulose acetate / ZIF-7 ethanol-water solvent, peak addition seems less significant. The XRD analysis showed that the higher the ZIF-7 concentration, the higher the value of the degree of crystallinity. This can also be confirmed by increasing the glass transition temperature (Tg) for each increase in the concentration of ZIF-7 based on the DSC analysis.

POSTER ABSTRACTS