



AFFPS 2019
The Asian Federation for Pharmaceutical Sciences

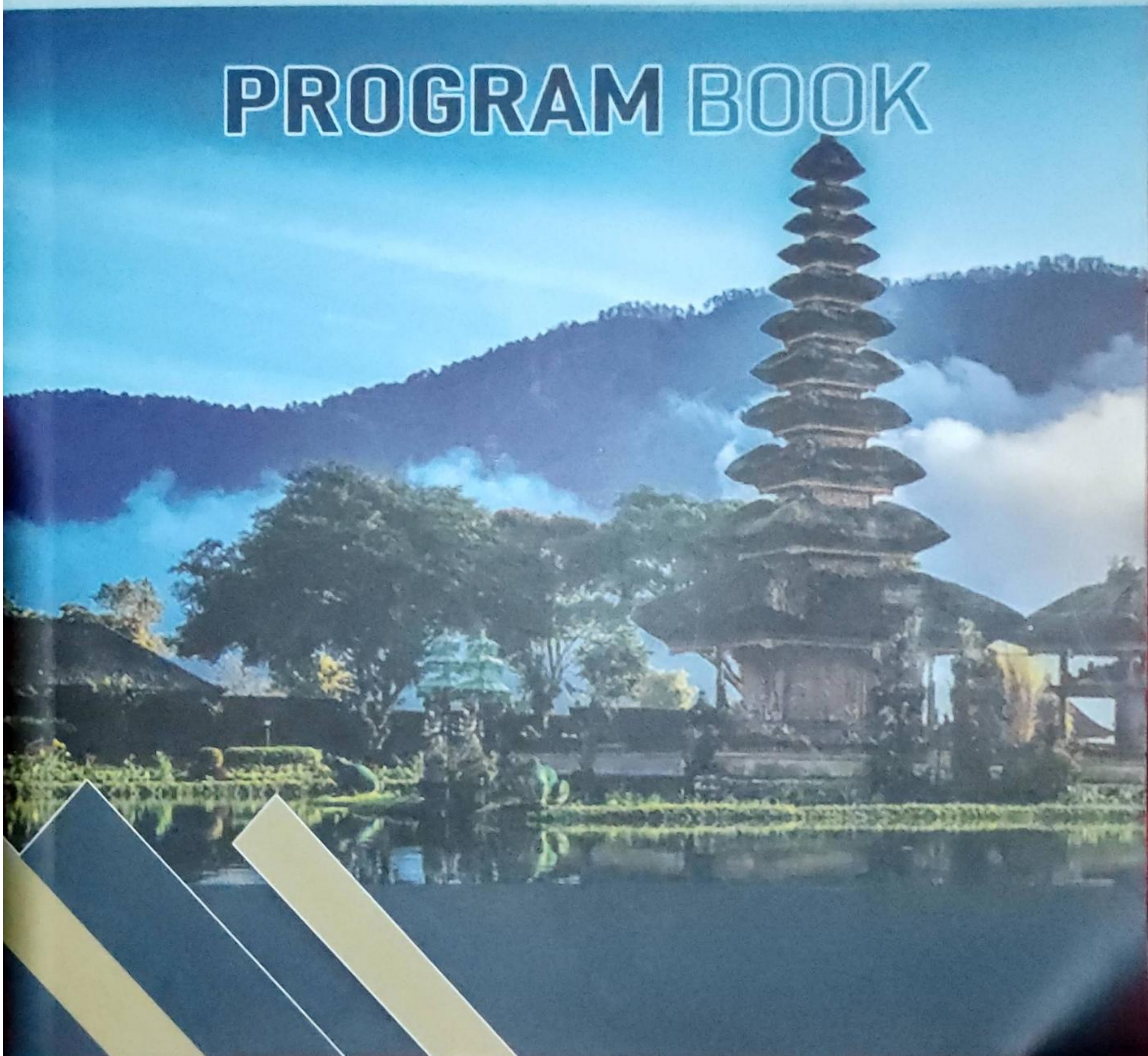
ICAPPS 2019
The 4th International Conference on Education Pharmacy and Pharmaceutical Sciences

**THE ROLE OF
PHARMACEUTICAL SCIENCES
IN THE EMERGING ERA OF
INDUSTRIAL REVOLUTION 4.0**

**PATRA JASA RESORT & VILLAS
BALI, INDONESIA**

OCTOBER 23RD - 27TH, 2019

PROGRAM BOOK



Patron
Steering Committee

Prof. Dr. rer. nat Rosari Saleh
Dr. Mahdi Jufri, M.Si., Apt.
Prof. Dr. Arry Yanuar, M.Si., Apt.
Prof. Dr. Abdul Mun'im, M.Si., Apt.
Prof. Yahdiana Harahap, M.S., Apt.

Chair of The Organizing Committee
Chair of The Conference
Vice Chair

Prof. Dr. Berna Elya, M.Si., Apt.
1. Dr. Rani Sauriasari, M.Sc., Apt.
2. Dewa Ayu Swastini, M.Farm., Apt.

Treasurer

Chief
Staff

Rina Rahmawati, M.Farm., Apt.
1. Dian Mayasari, S.E.
2. Trisnawati
3. Dr. Novi Yantih, M.Si., Apt.

Secretary

Chief
Staff

Rosita Handayani, M.Si.
1. Kurnia Sari Setio Putri, M.Farm., Apt.
2. Ayun Erwina Arifianti, M.Farm., Apt.
3. Dr. Ratika Rahmasari, M.Pharm.Sc., Apt.
4. Annisa Zahra, S.Farm.

Publication, Documentation, Information and Technology

Chief
Staff

Suryadi, S.Kom
1. Egi Yudha, A.Md
2. Aprilanda Dwisuna, A.Md
3. Wisnu Pratikto
4. Putu Sanna Yustiantara, M.Si., Apt.

Logistic

Chief
Staff

Rezi Riadhi Syahdi, M.Farm.
1. Catur April Lianti, A.Md
2. Septiana Kuswari, S.E.
3. Mista
4. Ni Made Widiastuti, M.Si., Apt.
5. Made Krisna Adi Jaya, S. Farm., M. Farm., Apt.

Transportation

Chief
Staff

Dr. Heri Setiawan, M.Sc., Apt.
Anak Agung Rai Yadnya Putra, M.Si., Apt.

Sponsorship

Chief
Staff

Prof. Dr. Abdul Mun'im, M.Si., Apt.
1. Prof. Dr. Harmita, Apt.
2. Nuriza Ulul Azmi, M.Sc., Apt.
3. Marina Ika Irianti, M.Sc., Apt.

Event

Chief

Staff

Scientific Committee

Chief

Staff

4. Widya Dwi Aryati, M.Si., Apt.

: 6. I Wayan Martadi Santika, M.Si., Apt.

: 7. Cokorda Istri Sri Arisanti, M.Si., Apt.

: Baitha Palanggatan Maggadani, M.Farm., Apt.

: 1. Eme Stepani Sitepu, M.Sc., Apt

: 2. Larasati Arrum Kusumawardani, M.Si., Apt.

: 3. Widya Dwi Aryati, M.Si., Apt.

: 4. I Gusti Ngurah Jemmy Anton Prasetia, M.Si., Apt.

: 5. Ni Kadek Warditiani, M.Sc., Apt.,

: Dr. Fadlina Chany Saputri, M.Si., Apt.
(Universitas Indonesia)

: 1. Prof. Dr. Abdul Mun'im, M.Si., Apt.
(Universitas Indonesia)

2. Prof. Dr. Amarila Malik, M.Si., Apt.
(Universitas Indonesia)

3. Prof. Dr. Arry Yanuar, M.Si., Apt.
(Universitas Indonesia)

4. Prof. Dr. Maksum Radji, M.Biomed., Apt.
(Universitas Indonesia)

5. Dr. Raditya Iswandana, M.Farm., Apt.
(Universitas Indonesia)

6. Santi Purnasari, M.Si., Apt.
(Universitas Indonesia)

7. Dr. Anton Bahtiar, M.Biomed., Apt.
(Universitas Indonesia)

8. Dr. Silvia Surini, M.Pharm.Sc., Apt
(Universitas Indonesia)

9. Dr. Hayun, M.Si., Apt.
(Universitas Indonesia)

10. Dr. Retnosari Andrajati, M.S., Apt.
(Universitas Indonesia)

11. Dr. Herman Suryadi, M.Si., Apt.
(Universitas Indonesia)

12. Prof. Dr. Shirley Kumala, M.Biomed., Apt
(Pancasila University)

13. Dr. I Made Agus Gelgel Wirasuta, M.Si., Apt.
(Udayana University)

14. Prof. Dr. Heni Rachmawati, M.Si., Apt.
(Bandung Institute of Technology)

15. Prof. Dr. M. Yuwono, MS., Apt
(Airlangga University)

16. Prof. Dr. Zullies Ikawati, Apt.
(Gadjah Mada University)

04 | *OPENING REMARKS*

09 | *COMMITTEE*

PROGRAM OVERVIEW | **11**

ORAL SESSION-1 | **14**

16 | *ORAL SESSION-2*

18 | *POSTER
PRESENTATION-1*

*POSTER
PRESENTATION-2* | **20**

*POSTER
PRESENTATION-3* | **23**

25 | *KEYNOTE SPEECH*

26 | *PLENARY LECTURE*

INVITED LECTURE | **37**

LOCATION MAP | **58**

Docking Studies and Molecular Dynamics Simulation of Compounds Contained in *Kaempferia Galanga L.* to Lipoxxygenase (LOX) for Anti-Inflammatory Drugs

Supandi¹, Yeni¹, Lusi Putri Dwita²

¹ Laboratory of Pharmacochimistry, Faculty of Pharmacy and science, Universitas Muhammadiyah Prof. DR. HAMKA, Jakarta, 13460, Indonesia

² Laboratory of Pharmacology, Faculty of Pharmacy and science, Universitas Muhammadiyah Prof. DR. HAMKA, Ja-karta, 13460, Indonesia

Corresponding author: yeni@uhamka.ac.id

AFPS 2019
The Asian Federation for Pharmaceutical Sciences

ICAPPS 2019

INTRODUCTION

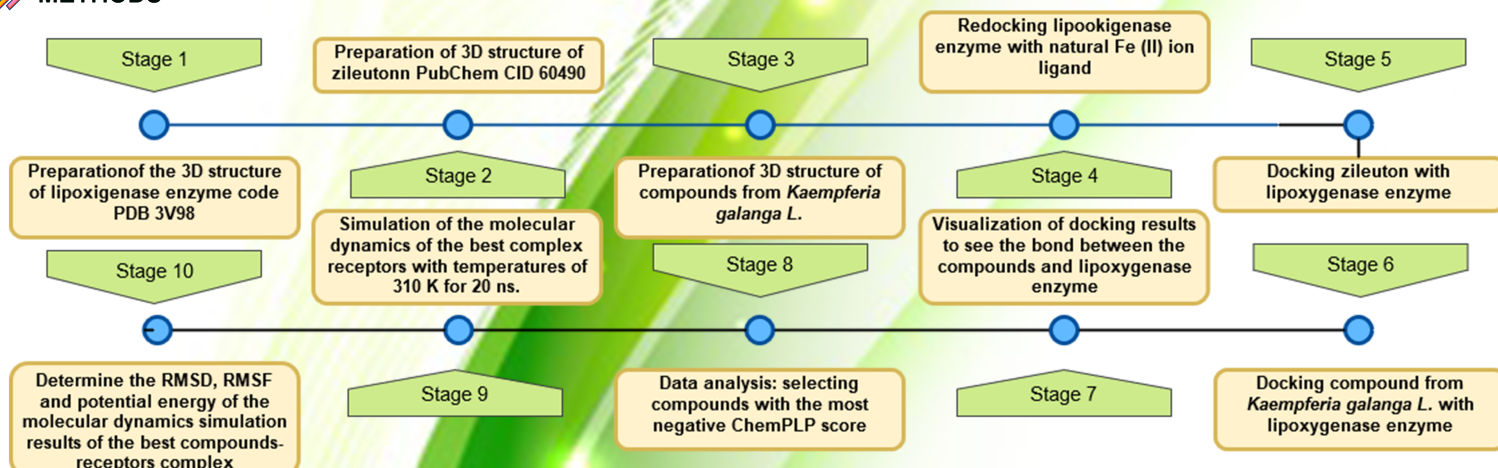


Inflammation is a self-protection response to begin the healing process. The goal is eliminating harmful stimuli, such as damaged cells, irritation and pathogens. However, the appeared symptoms in the form of redness, swelling, heat, pain and loss of function will interfere the body activities. Lipoxxygenase (LOX) is an enzyme that plays a role in the oxidation of Arachidonic Acid (AA) to leukotrienes (LTs), the potent pro-inflammatory mediators. *Kaempferia galanga L.* is a natural remedy that suspected of having anti-inflammatory activity potential. Docking studies that dominate computer-aided drug design (CADD) are conducted for virtual screening or optimization of drug screening and design. Docking studies between proteins and ligands can predict ligand orientation when bound to protein receptors or enzymes. Molecular dynamics simulations are used to understand the physical properties of the structure and function of biological macromolecules.

OBJECTIVES

The purposes of this study are predicting the activity of 21 compounds in *Kaempferia galanga L.*, namely ethyl cinnamate, ethyl p-methoxycinnamic acid, p-methoxycinnamic acid, 3-carene-5-one, camphene, δ -3-carene, p-methoxy styrene, γ -pinene, β -myrcene, p-cymene, 1,8-cineole, iso-myrcene, camphor, α -terpineol, p-cymene-8-ol, eucaryone, δ -cadinene, kaempferol, quercetin, cyanidin and delphinidin in inhibiting LOX and predicting the stability of ligand-LOX complex which has the greatest binding affinity.

METHODS

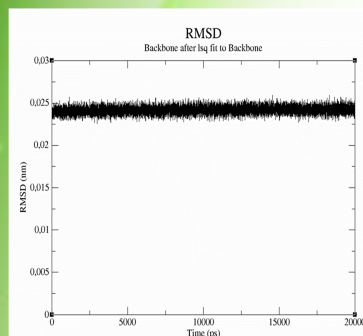


RESULTS AND DISCUSSION

The results of docking compounds from *Kaempferia galanga L.* and zileuton to 5-lipoxxygenase enzyme

No.	Compound	ChemPLP Score (kcal/mol)	No.	Compound	ChemPLP Score (kcal/mol)
1	Zileuton	-18,2282	12	1,8-cineole	-20,0000
2	Ethyl cinnamate	-19,9983	13	Iso-myrcene	-18,6944
3	Ethyl p-methoxycinnamic	-19,9923	14	Camphor	-20,0000
4	p-methoxycinnamic acid	-19,9995	15	α -terpineol	-19,9516
5	3-carene-5-one	-20,0001	16	p-cymene-8-ol	-18,7071
6	Camphene	-20,0000	17	Eucaryone	-20,0001
7	δ -3-carene	-20,0002	18	δ -cadinene	-19,8634
8	p-methoxy styrene	-19,9990	19	Kaempferol	-17,7609
9	γ -pinene	-20,0000	20	Quercetin	-16,9874
10	β -myrcene	-18,7074	21	Cyanidin	-13,3429
11	p-cymene	-19,0029	22	Delphinidin	-13,3238

Graph of RMSD on molecular dynamics simulations of δ -3-carene with 5-lipoxxygenase complex



CONCLUSION

The compound in *Kaempferia galanga L.* which has the greatest affinity in inhibiting the enzyme 5-lipoxxygenase (5-LOX) is δ -3-carene with the most negative ChemPLP value, -20,0002 kcal/mol. ChemPLP value of δ -3-carene shows its affinity for 5-LOX is greater than zileuton as a comparison drug. The stability of the δ -3-carene and LOX complex in molecular dynamics simulations showed stable result for 20 ns with RMSD and RMSF of no more than 3 Å and the average potential energy of -1.67392 x 10⁶ kcal/mol.

ACKNOWLEDGMENT

Special thanks to Ministry of Research, Technology and Higher Education of the Republic of Indonesia for the funding support and thanks to Universitas Muhammadiyah Prof. DR. HAMKA for the technical support and cooperation during conducting the research.

In the compounds docking result, there is 1 compound that has the greatest affinity, δ -3-carene with the lowest ChemPLP score, -20,0002 kcal/mol. ChemPLP value of δ -3-carene showed its affinity for 5-LOX is greater than zileuton as a comparison drug. It is possible that δ -3-carene has better anti-inflammatory activity compared to zileuton and can be used as a candidate for new anti-inflammatory drug with some further research, in vitro or in vivo research.

The stability of the ligand-receptor complex can be seen from the function of RMSD to the simulation time. The RMSD δ -3-carene with 5-lipoxxygenase complex in molecular dynamics simulations for 20 ns is no more than 3 Å. It indicated that the whole system shows good stability.

AFPS-ICAPPS in Bali, Indonesia
October 23-27, 2019



UNIVERSITAS
INDONESIA

Terpadu, Berkualitas, Berdaya

FAKULTAS

FARMASI

ICAPPS 2019
The 4th International Conference on Advance Pharmacy and Pharmaceutical Sciences

AFPS 2019
The Asian Federation for Pharmaceutical Sciences

Faculty of Pharmacy Universitas Indonesia and
The Asian Federation for Pharmaceutical Sciences (AFPS)
present this

Certificate of Appreciation

To:

Yeni

in recognition of the valuable contribution as:

Presenter in the Poster Session

in the 4th International Conference on Advance Pharmacy and Pharmaceutical Sciences (ICAPPS 2019)
in conjunction with the Asian Federation for Pharmaceutical Sciences (AFPS) Conference 2019
Patra Jasa Resort and Villas, Bali, Indonesia
October 23rd-27th, 2019

IAI Accreditation Number: 084/SK-SKP/PP.IAI/1822/I/2019

Plenary Speaker: 4.5 SKP, Invited Speaker: 4.5 SKP, Workshop Speaker: 6.5 SKP, Presenter of Oral/Poster Session: 3 SKP, Judges: 3 SKP,
Committee: 2.5 SKP, Workshop Participant: 6.5 SKP, Conference Participant: 10 SKP, Moderator: 1.5 SKP



Dr. Mahdi Jufri, M.Si., Apt.
Dean of Faculty of Pharmacy
Universitas Indonesia

Prof. Dr. Yahdiana Harahap, M.Si., Apt
President-Elect of Asian Federation for
Pharmaceutical Sciences