QUANTITATIVE STRUCTURE-ACTIVITY RELATIONSHIP (QSAR) OF *N'*-ETHYL-*N'*-PHENYL-*N*-BENZOYLTHIOUREA AND ITS DERIVATIVES AS ANTICANCER COMPOUNDS BY IN SILICO STUDY

D. Kesuma[1]*, Siswandono[2], and H. Santosa [1]
[1]Department of Pharmaceutical Chemistry, Faculty of Pharmacy, University of Surabaya.Raya Kalirungkut, Surabaya 60293, Indonesia
[2]Department of Pharmaceutical Chemistry, Faculty of Pharmacy, University of Airlangga.Dharmawangsa Dalam, Surabaya 60286, Indonesia

Email : dinikesuma@gmail.com

ABSTRACT

Quantitative Structure Activity Relationship (QSAR) has important role in drug development that is improving efficiency on next research to determine new derivatives which are more potent, safer, and have good absorption when consumed. In this research we used *N'*-Ethyl-*N'*-Phenyl-*N*-Benzoylthiourea and 12 derivatives which have anticancer activity based on *in silico* test. Then, we conducted their relationship analysis of physicochemical properties (lipophilic, electronic, and steric) to *in silico* prediction of activity, toxicity, and bioavailability to obtain the best QSAR equation. QSAR equation was determined by linear and non linier regression using statistic program of SPSS 20.0. The result showed that activity prediction (Log 1/RS, from docking on RR receptor PDB ID: 2EUD) with the best QSAR equation: Log $1/RS = 0{,}118$ Mw $+ 22{,}994$ pKa $+ 0{,}022$ tPSA^2 $- 2{,}590$ tPSA $-270{,}960$ ($n = 13$; $R = 0{,}949$; $SE = 2{,}054$; $F = 18{,}150$; $Sig = 0{,}000$), toxicity prediction (Log 1/LD-50, ACD/I-Lab prediction) with the best QSAR equation: Log $1/($LD-50 Mouse oral$) = - 4{,}527$ Mw $- 0{,}496$ tPSA^2 $+ 57{,}150$ tPSA $+ 744{,}724$ ($n = 13$; $R = 0{,}925$; $SE = 61{,}569$; $F = 17{,}846$; $Sig = 0{,}000$), and bioavailability prediction (Log1/F, ACD/I-Lab prediction) with the best QSAR equation: Log $1/F = - 0{,}006$ Mw $- 0{,}003$ tPSA $- 2{,}554$ ($n = 13$; $R = 0{,}802$; $SE = 0{,}132$; $F = 9{,}006$; $Sig = 0{,}006$). Furthermore, all of the best equation can be used to develop new compounds as anticancer agent.

Keywords: QSAR, *N'*-Ethyl-*N'*-Phenyl-*N*-Benzoylthiourea, Anticancer, In Silico

1. Introduction

The development of new anticancer drugs is a very important need, given that cancer has become the leading cause of death worldwide after cardiovascular disease. The type of cancer that causes the highest death in Indonesian women is breast cancer (WHO, 2014). The high prevalence of cancer needs to be overcome with precautionary measures and prompt and appropriate treatment. Meanwhile, drugs that have long been used gradually become less effective (Kar, 2007) and there is a tendency for cancer cells to become resistant to anticancer drugs (Tibes and Mesa, 2011, Tartarone et al., 2013).

Thiourea is a compound containing sulfur and nitrogen atoms whose chemical structure is similar to urea compounds that have been used as anticancer, including hydroxyurea, nitrosourea and 5-fluorouracil (Mutschler, 1999). Li (2010) has also synthesized urea and thiourea derivatives, and proved that phenyltiourea derivatives: *N*-(5-chloro-2-hydroxybenzyl)-*N*-4-hydroxybenzyl)-*N′*-phenyltiourea have cytotoxic activity on MCF cells -7 ($IC_{50} = 0.03$ with a mechanism of action inhibiting EGFR ($IC_{50} = 0.08$ as well as HER-2 ($IC_{50} = 0.35$). Li's research results also concluded that thiourea compounds have more potent cytotoxic activity than urea.

The results of several studies of thiourea compounds became the rationale for designing drug candidates by modifying the structure of *N*-Ethyl-*N*-Phenyl-*N′*-Benzoylthiourea as a parent compound and substituting aromatic rings with various substituents using the Topliss approach model. The reagents used were *N*-Ethyl-*N*-Phenylthiourea and benzoyl chloride derivatives with varied substituents of 2-Cl; 3-Cl; 4-Cl; 2,4-diCl; 3,4-diCl;

4-Br; 4-F; 4-NO2; 4-CH$_3$; 4-OCH$_3$; 4-CF$_3$; 4-t-butyl and H as an effort to improve lipophic and electronic properties.

Prediction of the interaction of pharmacophore groups with receptors was observed by in silico test so that it can be predicted the activity of the designed compound. Activity is indicated by the bond energy price / Rerank Score (RS). The smaller the price of bond energy shows the bond produced is more stable, so it is predicted that the activity will be greater (Hincliffe, 2008). Another aspect that needs to be considered is the permeability aspect, namely the ability of compounds to penetrate biological membranes. Lipinski suggested the Rules of Five as a condition that compounds have good permeability and can penetrate cell membranes. To provide information about the biological activity of a compound by using a method that is the Quantitative Structure-Activity Relationship (HKSA). Physical and chemical properties parameters determined in the HKSA are log P, ClogP, and tPSA values that describe lipophilic properties. Etot and pKa values that describe electronic properties. MR and CMR values that describe steric properties. Toxicity Parameters: LD-50 value and Bioavailability Parameter: F value (Siswandono, 2016).

Molecular modeling of *N*-Ethyl-*N*-Phenyl-*N′*-Benzoylthiourea compounds and their derivatives by docking with the 2EUD code and Ribonucleotide Reductase (RR) receptor obtained from Protein Data Bank (www.rcsb.org/pdb/home/home.do). Ribonucleotida Reductase receptor (2 EUD) was chosen because it is a receptor of gemsitabin (Xu, 2006). Gemsitabin is an anticancer drug whose mechanism of action is similar to Hydroxyurea (Avendano, 2008). As a comparison compound for the in

silico test Hydroxyurea, an anticancer compound that has been used clinically

From the results of predictions on the physical chemical properties (lipophilic, electronic, and steric), bioavailability, toxicity of the *N*-Ethyl-*N*-Phenyl-*N'*-Benzoylthiourea compound and its 12 derivatives, then look for quantitative structure-activity relationships, both linear or non-linear by using SPSS software so that the HKSA equation is then obtained. The best HKSA equation can be used as a reference for the development of new anticancer drugs.
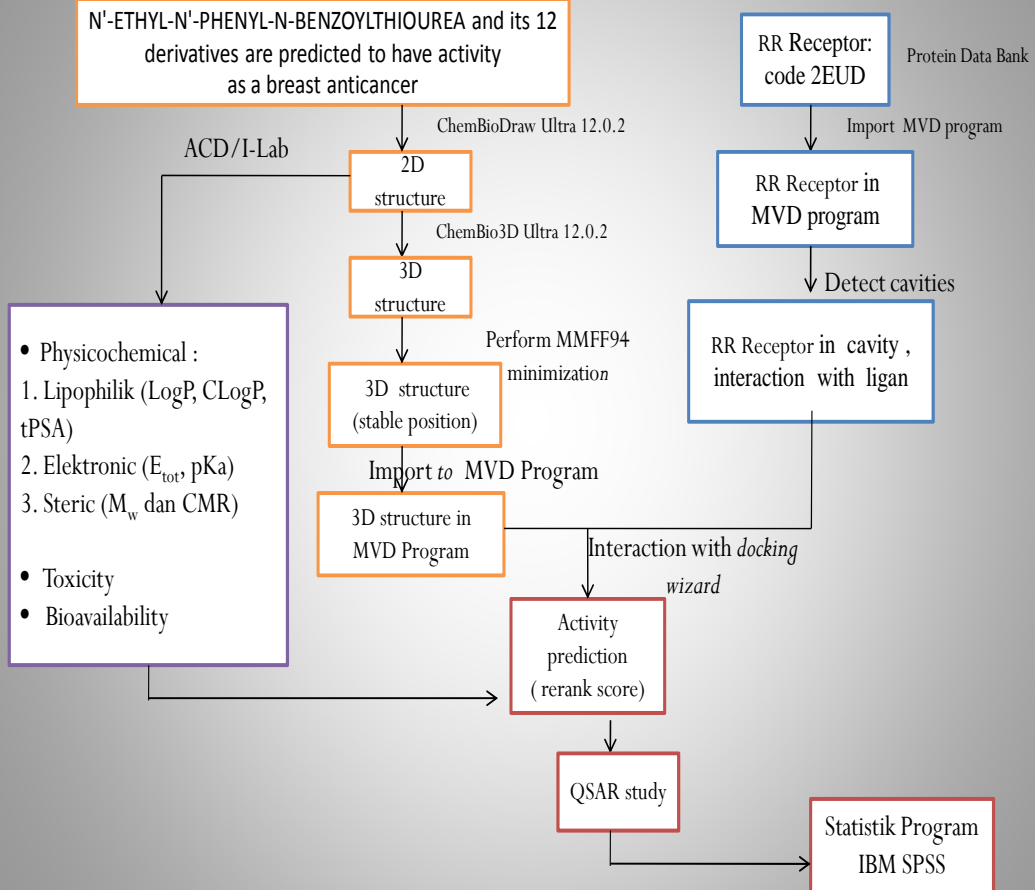
2. Materials Research :

Receptor Structure : RR (Protein Data Bank : 2EUD), 2D Structure **:** *N'*-ETHYL-*N'*-PHENYL-*N*-BENZOYLTHIOUREA   and   12   derivatives (ChemBioDraw Ultra 12.0.2, CambridgeSoft®), 3D stucture : *N'*-ETHYL-*N'*-PHENYL-*N*-BENZOYLTHIOUREA and 12 derivatives (ChemBio3D Ultra 12.0.2, CambridgeSoft®)
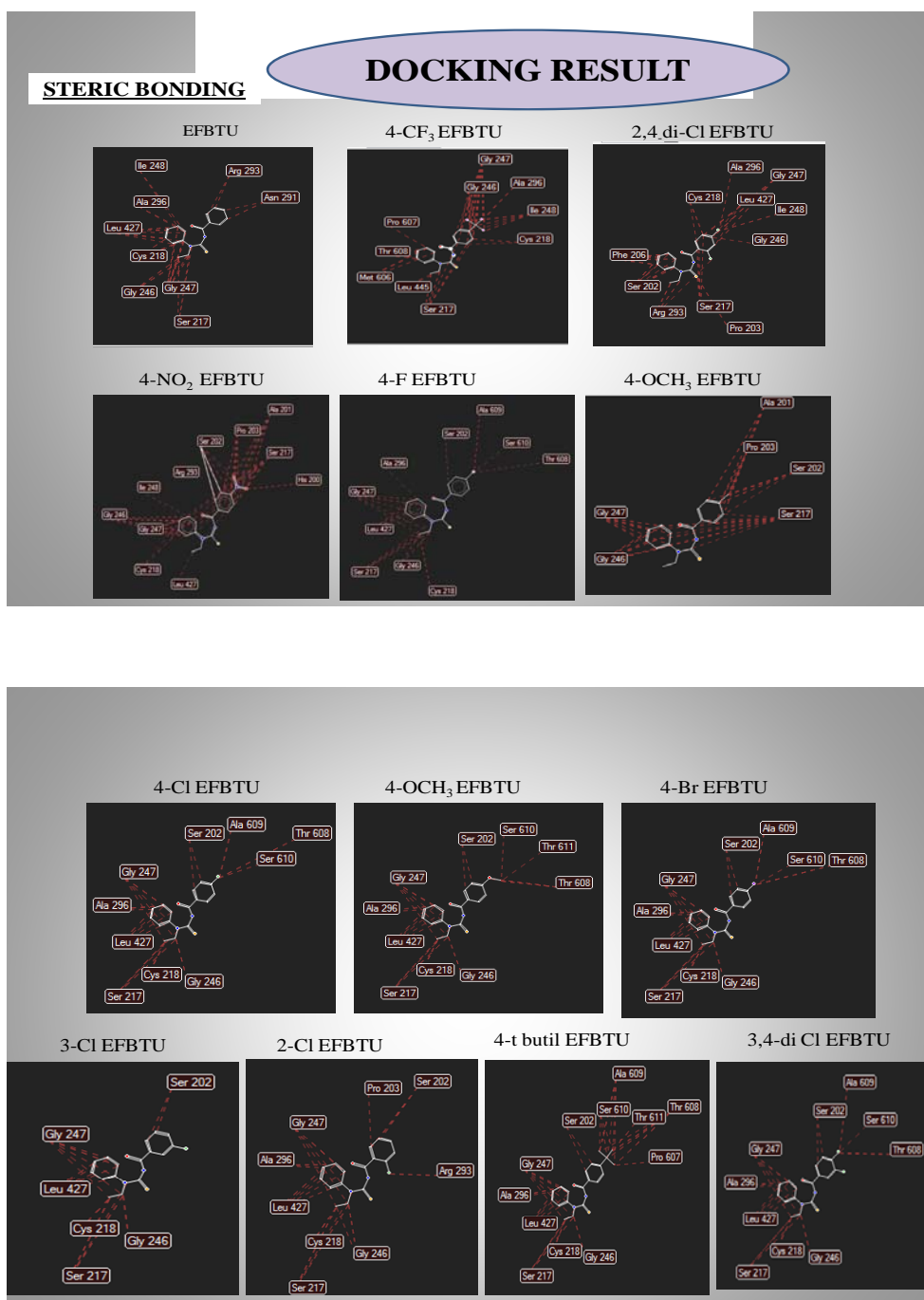
3. Research Tools

- Computer Intel Core i5-M430 2.27 GHZ, 2GB DDR 3, Window*s* 7 32 bit.

- Molegro Virtual Docker 5 (Molegro ApS)

- ChemBioDraw Ultra 12.0.2 (CambridgeSoft ®)

- ChemBio3D Ultra 12.0.2 (CambridgeSoft ®)

- ACD/I-Lab (Https://ilab.acdlabs.com/iLab2/)

- Statistic IBM SPSS® 21 (IBM Corp)

WORK SCHEME

N'-ETHYL-N'-PHENYL-N-BENZOYLTHIOUREA and its 12 derivatives are predicted to have activity as a breast anticancer

RR Receptor: code 2EUD

Protein Data Bank

ChemBioDraw Ultra 12.0.2

ACD/I-Lab

Import MVD program

2D structure

RR Receptor in MVD program

ChemBio3D Ultra 12.0.2

Detect cavities

3D structure

RR Receptor in cavity, interaction with ligan

Perform MMFF94 minimization

- Physicochemical :
1. Lipophilik (LogP, CLogP, tPSA)
2. Elektronic (E_{tot}, pKa)
3. Steric (M_w dan CMR)

- Toxicity
- Bioavailability

3D structure (stable position)

Import *to* MVD Program

3D structure in MVD Program

Interaction with *docking wizard*

Activity prediction (rerank score)

QSAR study

Statistik Program IBM SPSS

4. Result and Discussion

DOCKING RESULT

STERIC BONDING
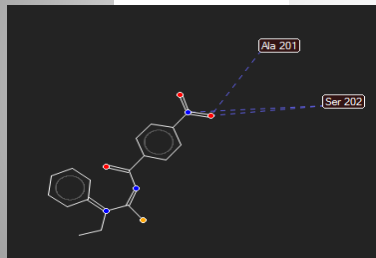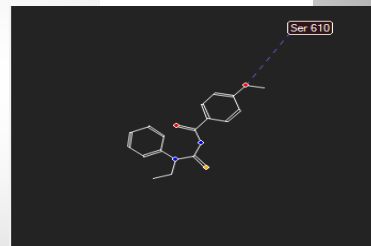
HYDROGEN BONDING

4-NO$_2$ EFBTU

4-OCH$_3$ EFBTU

Amino Acid Bonding with Ligan Compound

Com pounds	Ala 609	Ser 610	Thr 608	Pro 203	Ala 201	Pro 607	Met 606	Leu 445	Phe 206	Phr 611	Ile 248	Ala 296	Leu 427	Cys 218	Gly 246	Gly 247	Ser 217	Asn 291	Arg 293	Leu 427	Ser 202
1	-	-	-	-	-	-	-	-	-	-	2S	2S	6S	3S	2S	6S	3S	2S	2S	-	-
2	-	-	3S	-	-	1S	3S	2S	-	-	5S	2S	-	2S	4S	10S	5S	-	-	-	-
3	-	-	-	1S	-	-	-	-	4S	-	1S	1S	2S	2S	1S	3S	3S	-	3S	-	5S
4	-	2H 3S	-	-	-	-	-	-	-	-	-	1S	-	-	2S	5S	1H5S	-	2H2S	5S	-
5	4S	1S	1S	-	-	-	-	-	-	-	-	1S	-	1S	2S	5S	3S	-	-	5S	1S
6	-	-	-	2S	3S	-	-	-	-	-	-	-	-	-	5S	6S	9S	-	-	-	4S
7	1S	1S	1S	-	-	-	-	-	-	-	-	2S	5S	1S	1S	4S	2S	-	-	-	2S
8	-	1H 1S	2S	-	-	-	-	-	-	1S	-	2S	5S	1S	1S	4S	2S	-	-	-	2S
9	1S	1S	-	-	-	-	-	-	-	-	-	2S	5S	1S	1S	4S	2S	-	-	-	2S
10	-	-	-	1S	-	-	-	-	-	1S	-	-	5S	1S	2S	5S	4S	-	-	-	2S
11	-	-	-	-	-	-	-	-	-	-	-	2S	5S	1S	2S	4S	3S	-	1S	-	2S
12	4S	1S	4S	-	-	1S	-	-	-	-	-	2S	-	1S	1S	5S	2S	-	-	6S	5S
13	1S	1S	1S	-	-	-	-	-	-	-	-	2S	5S	1S	1S	4S	2S	-	-	-	2S

No.	COMPOUNDS	LIPOPHILIC PARAMETERS			ELECTRONIC PARAMETERS		STERIC PARAMETERS	
		Log P	C Log P	tPSA	Etot (kcal/mol)	pKa	Mw	CMR
1	EFBTU	4,43	3,348	32,34	27,0427	8,5	284,38	8,72
2	4-OCH$_3$	4,3	3,267	41,57	28,0975	8,3	314,4	9,3369
3	2-Cl	4,99	4,061	32,34	21,5375	8	318,82	9,2114
4	2,4-di Cl	5,55	4,774	32,34	12,9038	7,9	353,27	9,7028
5	3-Cl	4,99	4,061	32,34	16,6735	8,3	318,82	9,2114
6	4-NO$_2$	2,88	3,091	84,15	58,7802	8,2	329,37	9,3315
7	3,4-di Cl	5,55	4,654	32,34	25,611	8,2	353,27	9,7028
8	4-F	4,59	3,491	32,34	24,0975	8,4	302,37	8,7355
9	4-CH$_3$	4,92	3,847	32,34	27,036	8,5	298,4	9,1838
10	4-Cl	4,99	4,061	32,34	25,488	8,4	318,82	9,2114
11	4-CF$_3$	5,35	4,231	32,34	52,3485	8,3	352,37	9,2303
12	4-Br	5,26	4,211	32,34	26,1364	8,4	363,27	9,497
13	4-t butil	6,14	5,174	32,34	43,4906	8,5	340,48	10,5752

NO.	COMPOUNDS	RS (RERANK SCORE)	Toxicity LD-50 (mg/kg)		Bioavailability (F >70%) Oral
			Mouse (oral)	Rat (oral)	
1	EFBTU	-102.36	800	650	0,590
2	4-OCH$_3$	-112.70	840	500	0,590
3	2-Cl	-108.84	600	580	0,590
4	2,4-di Cl	-107.49	500	790	0,205
5	3-Cl	-106.04	600	580	0,205
6	4-NO$_2$	-105.83	550	750	0,167
7	3,4-di Cl	-104.80	570	320	0,205
8	4-F	-102.34	670	340	0,590
9	4-CH$_3$	-102.21	770	480	0,629
10	4-Cl	-100.60	600	580	0,205
11	4-CF$_3$	-97.76	390	300	0,205
12	4-Br	-96.43	380	530	0,205
13	4-t butil	-93.31	620	700	0,205

LIPINSKI RULE OF FIVE

No	Compound	BM	Log P	H donor	H aceptor
		<500	<5	<5	<10
1	EFBTU	284,38	2,68	1	3
2	4-OCH$_3$	314,40	3,48	1	4
3	2-Cl	318,82	3,48	1	3
4	2,4-di Cl	353,27	4,11	1	3
5	3-Cl	318,82	4,11	1	3
6	4-NO$_2$	329,37	2,60	1	6
7	3,4-di Cl	353,27	4,74	1	3
8	4-F	302,37	3,53	1	3
9	4-CH$_3$	298,40	3,77	1	3
10	4-Cl	318,82	4,07	1	3
11	4-CF$_3$	352,37	3,58	1	3
12	4-Br	363,27	4,25	1	3
13	4-t butil	340,48	5,00	1	3

Correlation Matrix

No.	Physico chemical Parameters	Correlation	Rerank Score	LD-50 Mouse Oral	LD-50 Rat oral	F > 70%
1	log P	*Pearson Correlation*	0,458	-0,293	-0,184	-0,234
		Sig. (2tailed)	0,115	0,331	0,548	0,442
2	C log P	*Pearson Correlation*	0,418	-0,506	0,022	-0,541
		Sig. (2tailed)	0,156	0,077	0,944	0,056
3	tPSA	*Pearson Correlation*	-0,248	-0,033	0,371	-0,214
		Sig. (2tailed)	0,414	0,915	0,211	0,482
4	Etot	*Pearson Correlation*	0,367	-0,227	-0,015	-0,297
		Sig. (2tailed)	0,217	0,456	0,962	0,325
5	pKa	*Pearson Correlation*	0,602*	0,352	-0,242	0,196
		Sig. (2tailed)	0,029	0,239	0,425	0,522
6	Mw	*Pearson Correlation*	0,282	-0,844**	-0,033	-0,774**
		Sig. (2tailed)	0,351	0,000	0,915	0,002
7	CMR	*Pearson Correlation*	0,338	-0,289	0,311	-0,547
		Sig. (2tailed)	0,259	0,339	0,301	0,053

Regression Analysis Result Dependent Variable : Rerank Score

QSAR equation (1 parameter):

Log 1/RS = 17,138 pKa – 245,378

(n = 13; R = 0,602; SE = 4,44163; F = 6,253; Sig = 0,029)

QSAR equation (2 parameters):

Log 1/RS = 0,137 Mw + 24,362 pKa – 350,158

(n = 13; R = 0,832; SE = 3,23804; F = 11,231; Sig = 0,003)

QSAR equation (3 parameters):

Log 1/RS = 0,118 Mw + 22,994 pKa + 0,022 tPSA^2 – 2,590 tPSA – 270,960

(n = 13; R = 0,949; SE = 2,0598; F = 18,150; Sig = 0,000)

Regression Analysis Result Dependent Variable : LD-50 Mouse Oral

QSAR equation (1 parameter):

Log 1/LD-50 Mouse oral = -4,867 Mw + 2197,306

(n = 13; R = 0,844; SE = 78,7795 ; F = 27,200; Sig = 0,000)

QSAR equation (2 parameters):

Log 1/LD-50 Mouse oral = -4,527 Mw – 0,496 tPSA^2 + 57,150 tPSA + 744,724

(n = 13; R = 0,925; SE = 61,56984; F = 17,846; Sig = 0,000)

QSAR equation (3 parameters):

Log 1/ LD-50 Mouse oral = -4,479 Mw – 0,518 Etot – 0,491 tPSA^2 + 56,889 tPSA + 746,808

(n = 13; R = 0,926; SE = 64,99560; F = 12,030; Sig = 0,002

Regression Analysis Result Dependent Variable : Bioavailability

QSAR equation (1 parameter):

Log 1/F = -0,006 Mw + 2,447

(n = 13; R = 0,774; SE = 0,13352; F = 16,416; Sig = 0,002)

QSAR equation (2 parameters):

Log 1/F = -0,006 Mw – 0,003 tPSA – 2,554

(n = 13; R = 0,802; SE = 0,13209; F = 9,006; Sig = 0,006)

QSAR equation (3 parameters):

Log 1/F = -0,007 Mw – 0,200 pKa – 0,003 tPSA + 4,434

(n = 13; R = 0,819; SE = 0,13367; F = 6,118; Sig = 0,015)

5. Conclusion

The best QSAR equation (RS, LD-50, and F) :

Log 1/RS = 0,118 Mw + 22,994 pKa + 0,022 $tPSA^2$ – 2,590 tPSA -270,960
(n = 13; R = 0,949; SE = 2,054; F = 18,150; Sig = 0,000)

Log 1/(LD-50 Mouse oral) = - 4,527 Mw – 0,496 $tPSA^2$ + 57,150 tPSA + 744,724

 (n = 13; R = 0,925; SE = 61,569; F = 17,846; Sig = 0,000)

Log 1/F = - 0,006 Mw - 0,003 tPSA – 2,554

(n = 13; R = 0,802; SE = 0,132; F = 9,006; Sig = 0,006)

6. References

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2nd Bandung International Conference on Medicinal Chemistry (ICMC 2017)

Institut Teknologi Bandung
Indonesia

5-6 October 2017

2nd Bandung
International Conference
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Abstract Book

Welcome to Bandung

PREFACE

The 2ⁿᵈ Bandung International Conference on Medicinal Chemistry (BICMC-2) is an international conference dedicated to promoting advances in medicinal chemistry as the gateway to discover novel drugs. Previous successful meetings, the first BICMC (2009) has motivated us to reorganize this conference, and still aims to improve together with stimulate international scientific exchange and collaboration.

The developments of science and technologies in the field of pharmacy seek to shorten the time of study and reduce the costs required, by staying to prioritize the findings of new drugs that are safe, efficacious and of high quality. Medicinal chemistry plays an important role as a science of novel drugs discovery. To support the efforts toward generating drug discovery, there is a need to improve the quality of teaching and research in the field of medicinal chemistry. The required efforts include the exchange of information on medical chemistry systems and learning materials; dissemination of research results and improvement of its quality; as well as education from world-renowned medical chemists.

With the intention of bridging the important role of medical chemistry in the development of pharmaceutical science and technology, School of Pharmacy ITB in collaboration with the Indonesian Society of Medicinal Chemistry (ISMC) intend to organize "The 2ⁿᵈ Bandung International Conference on Medicinal Chemistry 2017 (BICMC-2 2017)".

The conference covers topics of pharmaceutical chemistry such as new synthetic method, novel drug targets, new strategies for drug discovery including analytical, high-throughput medicinal and combinatorial advances, lead identification and optimization, as well as the role and significance of preclinical studies in drug development. The scientific programs include plenary and invited lectures to highlight some of major developments in medicinal chemistry especially in the scope of pharmaceutical science and technology. Furthermore, this conference is designed to facilitate scientists and professionals to broaden their research as well as social network through oral and poster presentation. In order to spread the conference outcomes, selected papers will be published in a SCOPUS-indexed journal such as Journal of Mathematical and Fundamental Sciences.

After all, for the second BICMC 2017, organizing committee would thank the Rector of ITB, the Dean of School of Pharmacy ITB, and The Indonesian Society of Medicinal Chemistry (ISMC) for supports and collaboration. We would also like to express gratitude to the participants as well as sponsors, such as PT. Bio Farma (Persero), PT. Nutrifood Indonesia and others who have well contributed in BICMC 2017.

Once again, welcome to BICMC 2017! We wish you have a pleasant and wonderful stay in Bandung, Indonesia!

Sincerely yours,

Assoc. Prof. Rahmana E. Kartasasmita
Chairman

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SCHEDULE OF THE CONFERENCE

Date	Time	Schedule
Thursday, October 5th 2017	07.30 – 08.30	Registration
	08.30 – 09.00	Opening Ceremony : Culturel Performance Opening remarks : • Chairman report: Dr.rer.nat Rahmana E. Kartasasmita • The president of ISMC: Assoc. Prof. Arry Yanuar • Dean of School of Pharmacy ITB: Prof. Daryono H. Tjahjono • Rector of ITB : Prof. Ir. Kadarsah Suryadi, DEA Photo session of all participants
	09.00–09.45	**Keynote Speech : Dra. Maura Linda Sitanggang, Ph.D** (Director General of Pharmaceutical and Medical Devices, Ministry of Health)
	09.45-10.00	*Coffee break / Poster Session and Exhibition*
		Moderator : Prof. Daryono Hadi Tjahjono
	10.00-11.00	**Plenary Lecture 1: Prof. Tomohiko Ohwada** (Laboratory of Organic and Medicinal Chemistry, Graduate School of Pharmaceutical Sciences, The University of Tokyo)
	11.00-12.00	**Plenary Lecture 2: Prof. Jeewoo Lee** (Seoul National University, South Korea)
	12.00-13.00	*Lunch break / Poster Session and Exhibition*

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Date	Time	Schedule		
		Hall Room *Moderator : Assoc. Prof. Amir Musadad*	**Room A** *Moderator : Prof. Tutus Gusdinar*	**Room B** *Moderator : Assoc. Prof. Marlia Singgih Wibowo*
Thursday, October 5th 2017	13.00-13.30	**Invited speaker 1:** **Assoc. Prof. Arry Yanuar**	**Invited speaker 3:** **Prof. Siswandono**	**Invited speaker 5:** **Assist. Prof. Supat Jiranusornkul**
	13.30-14.45	Oral 1: OP-16, OP-17, OP-26, OP-31, OP-32	Oral 2: OP-11, OP-25, OP-02, OP-06, OP-14	Oral 3: OP-03, OP-28, OP-33, OP-34, OP-30
	14.45-15.15	*Coffee break / Poster Session and Exhibition*		
		Hall Room *Moderator : Assist Prof. Elin Julianti*	**Room A** *Moderator : Assoc. Prof. Rahmana E. Kartasasmita*	**Room B** *Moderator : Assoc. Prof. Arry Yanuar*
	15.15-15.45	**Invited speaker 2:** **Assoc. Prof. Ly Le**	**Invited speaker 4:** **Assoc. Prof. Ritmaleni**	**Invited speaker 6:** **Assoc. Prof. Marcellino Rudyanto, Ph.D**
	15.45-17.00	Oral 4: OP-04, OP-05, PP-04	Oral 5: OP-07, OP-20, OP-21, OP-24	Oral 6: OP-19, OP-08, OP-15, OP-22

Date	Time	Schedule	
Friday, October 6th 2017	07.30 - 08.00	Registration	
		Moderator: Prof. Jutti Levita	
	08.00 – 09.00	**Plenary Lecture 3: Prof. Jonathan Baell** (Medicinal Chemistry, Monash Institute of Pharmaceutical Sciences; Co-Director, Australian Translational Medicinal Chemistry Facility)	
	09.00 – 09.15	*Coffee break / Poster Session and Exhibition*	
		Moderator: Dr.rer.nat Sophi Damayanti	
	09.15 - 10.15	**Plenary Lecture 4: Prof. Sun Choi** (Ewha Womans University, South Korea)	
	10.15 – 11.15	**Plenary Lecture 5: Prof. Lak Shin Jeong** (Seoul National University, South Korea)	
	11.15 – 13.30	*Lunch break / Poster Session and Exhibition*	
		Hall Room *Moderator: Assist Prof. Ilma Nugrahani*	**Room A** *Moderator: Dr. Benny Permana*
	13.30-14.00	**Invited Speaker 7: Prof. Jutti Levita**	**Invited Speaker 8: Assoc. Prof. Enade Perdana Istyastono**
	14.00-15.15	Oral 7: OP-09, OP-23, OP-27, OP-35, OP-01, OP-36	Oral 8: OP-10, OP-12, OP-13, OP-18, OP-29, OP-37
	15.15-15.45	Awards and Closing Ceremony	

DETAILED SCHEDULE OF THE CONFERENCE

THURSDAY, OCTOBER 5TH 2017
PLACE: HALL ROOM

Time	Activity
07.30	Registration
08.30	Opening of the conference
	- Cultural performance
	- Opening remarks
	- Photo session
09.00	Keynote speech
	Dra. Maura Linda Sitanggang, Ph.D
09.45	Coffee break| Poster session and exhibition
10.00	*Moderator: Prof. Daryono H. Tjahjono*
	Plenary speaker-1: Prof. Tomohiko Ohwada
	"Probing the Hydrophobic Binding Pocket of Lipid- Liganded G-Protein-Coupled Receptors"
11.00	Plenary speaker-2: Prof. Jeewoo Lee
	"Discovery of Transient Receptor Potential V1 Antagonist for Novel Analgesic Drugs"
12.00	Lunch| Poster session and exhibition

THURSDAY, OCTOBER 5TH 2017
PLACE: HALL ROOM

Time	Activity
	Moderator: Assoc Prof. Amir Musadad
13.00	**Invited speaker-1: Assoc. Prof. Arry Yanuar** "Virtual Screening and Molecular Dynamics Simulation of Compound from Herbal Database Indonesia Against Histone Deacetylase-2 (HDAC-2)"
13.30	**OP-16: Fauzan Zein Muttaqin** "Virtual Screening of DNA Topoisomerase II Alpha Inhibitor as Antileukemia from Natural Product Database Using Pharmacophore Modeling and Molecular Docking"
	OP-17: Riska Prasetiawati "Modification of Chalcone with Pyrazole Derivates as a Novel Compound Targeted Breast Cancer Using *In Silico* Study"
	OP-26: Syafrida Siregar "Fragment-Based Design, Computational ADMET, and Molecular Docking Studies of Novel Ibuprofen-Based Ligand as Inhibitor of Ebola Virus Glycoprotein"
	OP-31: Selvira Anandia Intan Maulidya "Structure-Based Virtual Screening for Identification of Potential HDAC8 Inhibitors"
	OP-32: La Ode Aman "Ligand and Structure-Based Pharmacophore Model of Curcumin Analog"
14.45	Coffee break| Poster session and exhibition

THURSDAY, OCTOBER 5TH 2017
PLACE: HALL ROOM

Moderator: Assist. Prof. Elin Julianti

15.15	Invited speaker-2: Assoc. Prof. Ly Le
	"Systems Pharmacology Approach in Drug Development"
15.45	OP-04: Nurul Auliasari
	"The Effect of Packaging AS-ODN Targeted EBA-175 Gene into Nanoparticles on The Inhibition of Schizont Growth"
	OP-05: Dina Permata Wijaya
	"The Efficient Delivery of AS-ODN Targeted DHS Gene Loaded Nanocarrier in Blocking Life Cycle of *Plasmodium falciparum*"
	PP-04: Farida Suhud
	"Synthesis and *in-Vitro* Activity of Para Substituted Compounds of 1-Benzyl-3-Benzoylurea as Antiproliferation"

THURSDAY, OCTOBER 5TH 2017
PLACE: ROOM A

Time	Activity
	Moderator : Prof. Tutus Gusdinar
13.00	**Invited speaker-3: Prof. Siswandono** "Molecular Modelling and QSAR of N-Benzoyl-N-Thiourea Derivatives as Anticancer Drug Candidate
13.30	**OP-11: Sabila Robbani** "Shelf-life of Antiatherosclerosis Herb Based on Bacterial Count and pH" **OP-25: Pramukti Nawar Ra'idah** "Secondary Metabolites from Leaves of *Cryptocarya pulchrinervia* (Lauraceae) and Their Antibacterial Activities" **OP-02: Dini Kesuma** "Quantitative Structure-Activity Relationship (QSAR) of N'-ethyl-N'-phenyl-N-benzoylthiourea and Its Derivatives as Anticancer Compounds by *In Silico* Study" **OP-06: Muhammad Hasan Bashari** "The Ethanol Extract of Marine Sponge (*Stylissa carteri*) Demonstrates Potential Anti-cancer Activity in Colon Cancer Cells" **OP-14: Edy Meiyanto** "Genistein in Combination with Doxorubicin Potently Induced Cytotoxic and Inhibited Migration of Metastatic Breast Cancer Cells"
14.45	Coffee break / Poster Session and Exhibition

2ⁿ Bandung
International Conference
ICMC
2017
on Medicinal Chemistry
4-6 October 2017

THURSDAY, OCTOBER 5ᵀᴴ 2017
PLACE: ROOM A

Moderator : Assoc. Prof. Rahmana E. Kartasasmita

15.15 **Invited speaker-4: Assoc. Prof. Ritmaleni**
"Analog of Curcumin and Tetrahydrocurcumin: Synthesis, Antibacterial and Antioxidant Activity"

15.45 **OP-07: Julia Nofadini**
"Anti-hyperglycemia Activity Test of Anti-atherosclerosis Herbs Extract in The Water Using *In Vivo* Method"

OP-20: Nyi Mekar Saptarini
"Drug Therapy Affect Cartilage Oligomeric Matrix Protein Levels in Patients of Rheumatoid Arthritis and Osteoarthritis"

OP-21: Dr. Muhammad Yanis Musdja, M.Sc.
"Activity Test on Healing of Burn Wound of Isolate Catechins of Gambir (*Uncaria Gambir* Roxb.) on White Rat (*Rattus norvegicus*) Male"

OP-24: Kholis Amalia Nofianti
"*In Vitro, In Vivo,* and *In Silico* Evaluation of Benzoxazin Compound as Anti-Platelet Agent"

THURSDAY, OCTOBER 5TH 2017
PLACE: ROOM B

Time	Activity
	Moderator: Assoc.Prof. Marlia Singgih Wibowo
13.00	Invited speaker-5: Assist. Prof. Supat Jiranusornkul "Comparative Molecular Modeling for Designed Zinc Finger Protein Interacting with HIV-1 integrase 2-LTR-Circle Junctions"
13.30	OP-03: Muhammad Arba "In Silico Study on The Interaction of Porphyrin Derivatives and B5 Subunit of 20s Proteasome"
	OP-28: Hubbi Nashrullah Muhammad "Interactions and Molecular Mechanism of Intercalation and Minor-Groove Binding of Porphyrin-Acridine to Duplex B-DNA"
	OP-33: Lina Nurfadhila "Study of Flavonoid Glycosides and Caffeonyl Acid Derivates of *Lonicera japonica* Thunb.: Cancer Activity Inhibition, Molecular Docking, and Molecular Dynamic" OP-34: Muhammad Yusuf "The Effect of pH to The Interaction Between Folic Acid and Folate Receptor Alpha: Molecular Dynamics Study" OP-30: Zenith Putri Dewianti "Quantitative Structure Activity Relationships, Molecular Docking, and Molecular Dinamic Study of Dehydroandrographolide and Andrographolide "
14.45	Coffee break / Poster Session and Exhibition

THURSDAY, OCTOBER 5TH 2017
PLACE: ROOM B

Moderator: Assoc. Prof. Arry Yanuar

15.15 Invited Speaker-6: Marcellino Rudyanto, Ph.D.
"Preparation of Vitamin A from Indonesian Lemongrass Oil"

15.45 OP-19: Tegar Achsendo Yuniarta
"Virtual Screening Study to Obtain Prolyl-tRNA Synthetase Inhibitors as Antimalarial Drug Candidates"

OP-08: Sabila Robbani
"Antioxidant Activity Assay of Anti-atherosclerosis Herbs Using DPPH Method"

OP-15: Rohmad Yudi Utomo
"Reveal Pro-oxidant Activity of PGV-0, PGV-1, and PGV-0 on HER2 Overexpressed Cancer Cells"

OP-22: Sonni Maurit Benu
"Three Pentacyclic Triterpenoids from Dischidia Nummularia"

FRIDAY, OCTOBER 6TH 2017
PLACE: HALL ROOM

Time	Activity
07.30	Registration
08.00	*Moderator: Prof. Jutti Levita*
	Plenary speaker-3: Prof. Jonathan Baell
	"Your Natural Product Contains a Promiscuous Pains Motif: Is It Useful as a Biochemical Probe or In Drug Discovery?"
09.00	Coffee break| Poster session and Exhibition
09.15	*Moderator: Assoc. Prof. Sophi Damayanti*
	Plenary speaker-4: Prof. Sun Choi
	"Elucidation of Protein Motion, Allostery, and Intra-Molecular Signaling of GPCR, and Its Application to Drug Discovery"
	Plenary speaker-5: Prof. Lak Shin Jeong
	"Drug Discovery Targeting Adenosine Receptor"
11.15	Lunch| Poster session and exhibition
15.15	Awards and Closing

FRIDAY, OCTOBER 6ᵀᴴ 2017
PLACE: HALL ROOM

Time	Activity
	Moderator: Assist. Prof. Ilma Nugrahani
13.30	**Invited Speaker-7: Prof. Jutti Levita** "Discovering Anti-inflammatory Agents: From *In Silico* Pharmacology To Animal Study"
14.00	**OP-09: Rimadani Pratiwi** "A New Synthetic Method of Water Soluble Pyrazoliumylporphyrin Using Methyl *p*-Toluenesulfonate" **OP-23: Fransiska Kurniawan** "*In Silico* Study, Synthesis, and Cytotoxicity Test of Porphyrin Derivatives as Candidate of Anticervical Cancer Agents"
	OP-27: Tri Widiandani "Molecular Modeling, Synthesis, and Antiproliferative Effect of 1-allyl-3-(3-chlorobenzoyl)thiourea and 1-allyl-3-(4-methoxybenzoyl)thiourea on MCF-7/Her2 Breast Cancer Cells"
	OP-35: Fadhila Utari "Antioxidant Activities of Bark, Leaves, Roots Extracts, and Secondary Metabolites from *Salix Tetrasperma* Roxb." **OP-01: Muhammad Hasan Bashari** "The *n*-Hexane Fraction of *Myrmecodia pendans* Inhibits Cell Proliferation and Survival in Breast Cells" **OP-36: Nadhirah binti Tahir** "Potential DENV NS2B/NS3 Protease Inhibitors: Biological Screening and Molecular Docking Approach On Malaysian Natural Products

Moderator: Dr. Benny Permana

13.30 Invited Speaker-8: Assoc. Prof. Enade Perdana Istyastono
"Potential Applications of PyPLIF in Structure-based Virtual Screening"

14.00 OP-10: Yuditya Artha Asideta Pohan
"Molecular Docking on HMG CoA Reductase Inhibitory Activity by Extracted Compounds from Melinjo (*Gnetum gnemon* L.) Seed"

OP-12: Indah Pratiwi
"*In Silico* Activity Analysis of Saponins and 2,5–Piperazinedione from Marine Organism against Procaspase-3 Activator"

OP-13: Febrina Amelia Saputri
"Interaction Study between Alpha-mangosteen, Beta-mangosteen, and Gamma-mangosteen with Cyclooxygenase Compared to Acetosal and Sc-558 AS "

OP-18: Muchtaridi Muchtaridi
"Bioassay-Guided Isolation, Identification, and Molecular Ligand-Target Insight of Neuraminidase Inhibitors from Fruits and Leaves of *Garcinia atroviridis*"

OP-29: Atika Marnolia
"*In Silico* Evaluation on Antiviral Activity of Alkaloid Compounds Through Molecular Docking Simulation Against Dengue Virus (DENV) NS5 Methyltransferase"

OP 37: Nurul Amira binti Nurul Azman
"Inhibitory Activity and Molecular Docking of Acetylcholinesterase Enzyme: Significant to Alzheimer Disease from *Cassia* sp."

LIST OF SPEAKERS

1	Keynote Speaker	**Dra. Maura Linda Sitanggang, PhD**
2	Plenary Speaker-1	**Prof. Tomohiko Ohwada**
		"Probing the Hydrophobic Binding Pocket of Liganded G-Protein-Coupled Receptors"
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		"Discovery of Transient Receptor Potential V1 Antagonist for Novel Analgesic Drugs
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		"Your Natural Product Contains a Promiscuous Pains Motif: Is It Useful as a Biochemical Probe in Drug Discovery?"
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		"Discovering Anti-inflammatory Agents: From *in Silico* Pharmacology to Animal Study"
14	Invited Speaker-8	**Assoc. Prof. Enade Perdana Istyastono**
		"Potential Application of PyPLIF in Structure-based Virtual Screening"

LIST OF ORAL PARTICIPANTS

1	OP-01	Muhammad Hasan Bashari	The N-Hexane Fraction of Myrmecodia Pendans Inhibits Cell Proliferation and Survival in Breast Cells
2	OP-02	Dini Kesuma	Quantitative Structure-Activity Relationship (QSAR) of N'-Ethyl-N'-Phenyl-N-Benzoylthiourea and Its Derivatives as Anticancer Compounds by *in Silico* Study
3	OP-03	Muhammad Arba	*In Silico* Study on The Interaction of Porphyrin Derivatives and B5 Subunit of 20s Proteasome
4	OP-04	Nurul Auliasari	The Effect of Packaging AS-ODN Targeted EBA-175 Gene into Nanoparticles on The Inhibition of Schizont Growth
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8	OP-08	Sabila Robbani	Antioxidant Activity Assay of Anti-Atherosclerosis Herbs Using DPPH Method
9	OP-09	Rimadani Pratiwi	A New Synthetic Method of Water Soluble Pyrazoliumylporphyrin using Methyl P-Toluenesulfonate
10	OP-10	Yuditya Artha Asideta Pohan	Molecular Docking nn HMG CoA Reductase Inhibitory Activity by Extracted Compounds From *Melinjo* (*Gnetum gnemon* L.) Seed
11	OP-11	Sabila Robbani	Shelf-Life of Antiatherosclerosis Herb Based on Bacterial Count and PH
12	OP-12	Indah Pratiwi	*In Silico* Activity Analysis of Saponins and 2,5–Piperazinedione From Marine Organism Against Procaspase-3 Activator
13	OP-13	Febrina Amelia Saputri	Interaction Study Between Alpha-Mangosteen, Beta-Mangosteen, and Gamma-Mangosteen With Cyclooxygenase Compared To Acetosal And Sc-558 as Oral Antiinflamation Drugs

14	OP-14	Edy Meiyanto	Genistein In Combination With Doxorubicin Potently Induced Cytotoxic and Inhibited Migration Of Metastatic Breast Cancer Cells
15	OP-15	Rohmad Yudi Utomo	Reveal Pro-Oxidant Activity of PGV-0, PGV-1, and PGB-0 on HER2 Overexpressed Cancer Cells
16	OP-16	Fauzan Zein Muttaqin	Virtual Screening Of DNA Topoisomerase II Alpha Inhibitor as Antileukemia From Natural Product Database Using Pharmacophore Modeling and Molecular Docking
17	OP-17	Riska Prasetiawati	Modification Of Chalcone With Pirazole Derivates as A Novel Compound Targeted Breast Cancer Using *in Silico* Study
18	OP-18	Muchtaridi Muchtaridi	Bioassay-Guided Isolation, Identification and Molecular Ligand-Target Insight of Nueraminidase Inhibitors From Fruits and Leaves of *Garcinia atroviridis*
19	OP-19	Nerdy	*In Vitro* Antinephrolitiatic Effect of Breadfruit (*Artocarpus altilis* (Park) Fosberg) Leaves Extract by Atomic Absorption Spectrophotometry
20	OP-20	Nyi Mekar Saptarini	Drug Therapy Affect Cartilage Oligomeric Matrix Protein Levels in Patients of Rheumatoid Arthritis and Osteoarthritis
21	OP-21	Dr. Muhammad Yanis Musdja, M.Sc	Activity Test on Healing of Burn Wound Of Isolate Catechins of *Gambir* (*Uncaria gambir* Roxb.) on White Rat (*Rattus norvegicus*) Male
22	OP-22	Sonni Maurit Benu	Three Pentacyclic Triterpenoids from *Dischidia nummularia*
23	OP-23	Fransiska Kurniawan	*In Silico* Study, Synthesis, and Cytotoxicity Test of Porphyrin Derivatives as Candidate of Anticervical Cancer Agents
24	OP-24	Kholis Amalia Nofianti	*In Vitro, in Vivo* and *in Silico* Evaluation of Benzoxazin Compound as Anti-Platelet Agent
25	OP-25	Pramukti Nawar Ra'idah	Secondary Metabolites from Leaves of *Cryptocarya pulchrinervia* (Lauraceae) and Their Antibacterial Activities
26	OP-26	Syafrida Siregar	Fragment-Based Design, Computational ADMET, and Molecular Docking Studies Of Novel Ibuprofen-Based Ligand as Inhibitor of Ebola Virus Glycoprotein

27	OP-27	Tri Widiandani	Molecular Modeling, Synthesis and Antiproliferative Effect of 1-Allyl-3-(3-Chlorobenzoyl)Thiourea and 1-Allyl-3-(4-Methoxybenzoyl)Thiourea on MCF-7/HER2 Breast Cancer Cells
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29	OP-29	Atika Marnolia	*In Silico* Evaluation on Antiviral Activity of Alkaloid Compounds Through Molecular Docking Simulation Against Dengue Virus (DENV) NS5 Methyltransferase
30	OP-30	Zenith Putri Dewianti	Quantitative Structure Activity Relationships, Molecular Docking, and Molecular Dinamic Study of Dehydroandrographolide and Andrographolide Derivatives as Novel Anti-Hepatitis B Virus Agents
31	OP-31	Selvira Anandia Intan Maulidya	Structure-Based Virtual Screening for Identification of Potential HDAC8 Inhibitors
32	OP-32	La Ode Aman	Ligand and Structure-Based Pharmacophore Model of Curcumin Analog
33	OP-33	Lina Nurfadhila	Study of Flavonoid Glycosides and Caffeonyl Acid Derivates of *Lonicera japonica* Thunb.: Cancer Activity Inhibition, Molecular Docking, and Molecular Dynamic
34	OP-34	Muhammad Yusuf	The Effect of PH To the Interaction Between Folic Acid and Folate Receptor Alpha: Molecular Dynamics Study
35	OP-35	Fadhila Utari	Antioxidant Activities of Bark, Leaves and Roots Extracts and Secondary Metabolites From *Salix Tetrasperma* Roxb.
36	OP-36	Nadhirah Binti Tahir	Potential DENV NS2B/NS3 Protease Inhibitors: Biological Screening and Molecular Docking Approach on Malaysian Natural Products
37	OP-37	Nurul Amira Binti Nurul Azman	Inhibitory Activity And Molecular Docking Of Acetylcholinesterase Enzyme: Significant To Alzheimer Disease From *Cassia* Sp.

LIST OF POSTER PARTICIPANTS

1	PP-01	Anceu Murniati	Isolation And Characterization Of Polyphenol Oxidase Extract in Rejected White Oyster Mushrooms (*Pleurotus ostreatus*)
2	PP-02	Pratama Anggi Saputra	ADME Property Prediction of The Chemical Constituents of *Physalis angulata* L. Plants and Their Interaction with The Macromolecular Targets of Anti-Inflammatory Agents
3	PP-03	Saeful Amin	Interaction Study of Dimethyilamilamine Doping Compound as Derivatization Result with Monomer The Framer of Molecular Imprinted Polymers (MIPS)
4	PP-04	Farida Suhud	Synthesis and *in-Vitro* Activity of Para Substituted Compounds of 1-Benzyl-3-Benzoylurea as Anti-proliferation
5	PP-05	Dona Fitria	Synthesis of Sildenafil Analogs as A Reference Standard for Testing of Traditional Medicine and Health Supplement's Product
6	PP-06	Carolina Tonggo Marisi Tambunan	Synthesis New Psychoactive Substances, Para-Methoxymethamphetamine (PMMA) from Meth-amphetamine as Reference Standard for Narcotics Analysis
7	PP-07	Anna Yuliana	Antibacterial Candidate of *Monascus* Pigments
8	PP-08	Widya Dwi Aryati	*In Silico* Prediction of Mutagenicity and Carcinogenicity of Colorants Used In Pharmaceutical Preparation
9	PP-09	Dadan Suryasaputra	Quantitative Structure-Activity Relationship and Molecular Docking Of Withanolide Secondary Metabolites Form Kecubung (*Datura Metel* L) as Agonists Glucocorticoid Receptor
10	PP-10	Rina Anugrah	Study Of The Potential Of Jackfruit Plant Flavonoids As Cyclooxygenase Inhibitors

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11	PP-11	Elsa Marlina	Molecular Docking And Molecular Dynamic Studies of Curcumin Derivative Compounds to MCL-1 Receptor and Their Toxicity Prediction
12	PP-12	Tia Widiawati	Virtual Screening Using Pharmacophore Modelling and Molecular Docking in Zinc Database Natural Product to Identify Potent Glucose Regulated Protein 78 (GRP78) Inducers
13	PP-13	Purnawan Pontana Putra	*In Silico* : Toxicity Prediction of Preservatives Using Software ADMET Predictor, QSAR Toolbox, Toxtree and Toxicity Estimation Software Tool (TEST)
14	PP-14	Welly Ratwita	Alpha Mangosteen Role in Glucose Tolerance Test
15	PP-15	Vienna Saraswaty	Endocarp of Melinjo (*Gnetum Gnemon*) Seed For Alternative Source of Antioxidant and Xanthine Oxidase Inhibitor
16	PP-16	Tedjo Narko	Effect of Kombucha Culture on Caffeine and Chlorogenic Acid Content In Fermentation of Robusta Green Coffee Beans (*Coffea Cenephora* L.)
17	PP-17	Mohammad Rizki Fadhil Pratama	Docking Study of Secondary Metabolites From *Glycyrrhiza Glabra* As PPAR-γ Agonists Similarity Over Affinity
18	PP-18	Diah Lia Aulifa	Pharmacophore Modelling and Molecular Docking of Phytoconstituents in *Angelica keiskei* for Alpha-Glucosidase Inhibitor Discovery
19	PP-19	Nuzul Wahyuning Diyah	*In Silico* Docking Study, Antimicrobial, and Cytotoxic Activity of Benzoylated N,N'-Dialkylurea
20	PP-20	Ruswanto	Synthesis and Characterization of Isonicotino-hydrazide Derivatives as Anti-Tuberculosis Candidate
21	PP-21	Nursamsiar	Interaction Study of Gossypol and Its Derivatives With B-Cell Lymphocytes 2 (BCL-2) Receptor
22	PP-22	Deden Indra Dinata	Blind Docking of Sesquiterpene Compounds Against Enzyme 5-Lipoxygenase and Its Toxicity Prediction

23	PP-23	Panditya Purnaya	New Microwave Assisted Method of 3-(4-Nitrophenyl)-2-Phenylquinazolin-4(3h)-One and 4-(4-Oxo-2-Phenylquinazolin-3(4h)-Yl)Benzenesulfonic Acid Synthesis
24	PP-24	Bina Lohita Sari	Structure-Based Virtual Screening of Zinc Natural Product Database to Identify Potential Lead Of Urokinase Plasminogen Activator (Upa)
25	PP-25	Kinanti Khansa Chavarina	Virtual Screening and Molecular Dynamics Simulation of Secondary Metabolites Derived From Marine Fungi as Vascular Endothelial Growth Factor Receptor (VEGFR2) Kinase Inhibitors
26	PP-26	Nita Rusdiana	The Use Pattern Of Household and Cosmetics Products by Public In Indonesia
27	PP-27	Kurnia Permadi	Interactional Study Compounds Contain In Pomegranate (*Punica Granatum* L) Peel With *Mycobacterium Tuberculosis* Enzymes As Antituberculosis Agent
28	PP-28	Catur Riani	Production of Soluble Reteplase in Escherichia Coli Using PET24b Expression Vector
29	PP-29	Ni Made Pitri Susanti	In Silico Anti Aterosclerosis Activity of Andrographolide From Sambiloto (*Andrographis paniculata* (Burm. F Ness)
30	PP-30	Dwi Syah Fitra Ramadhan	Quantitative Structure-Activity Relationships of Novel Phenyl Benzimidazoles as WNT/B-Catenin Inhibitor for Treatment Pancreatic Ductal Adenocarcinoma
31	PP-31	Dwi Utami	Screening, Characterization and Formation Dynamic of some Non-Steroidal Anti-Inflammatory Drugs (NSAIDS)-L-Proline Zwitterionic Co-Crystal
32	PP-32	Fitri Rochmahdian	QSAR Study of Novel Dithiocarbamate-Chalcone Derivates as Antiproliferative

33	PP-33	H. Muhammad Nur Abdillah	Study *in Silico* Molecular Docking and Toxicity Prediction of Vemurafenib Derivate Against Targeted Molecule Melanoma Inhibitory Activity (MIA) as An Antimelanoma (Skin Cancer)
34	PP-34	Benita Rachel Praevina N	Development Of Pineapple Stem Waste Xylan-5-Asa Prodrug For Colon Targeting
35	PP-35	Tovani Sri	Immunomodulator Activity of Ciplukan Leaf (*Physalis angulata* L.) and Vetiver Root (*Vetiveria zizanioides* L.) Extracts and Its Effect on Animal Model of Rheumatoid Arthritis
36	PP-36	Noor Erma Nasution Sugijanto	Chitosan Extracted From Flower Crab (*Portunus pelagicus*) Shell Waste
37	PP-37	Eldi Soraya Choirunissa	Application of Box-Behnken Design in Optimization of Surface Modified Chitosan-Acemannan Lipid Nanoparticles as Rifampicin Delivery System
38	PP-38	Tri Suciati	A Novel Vehicle of *Centela asiatica* Ethanolic Extract in Microparticle Based Chitosan Matrix for Promoting Fibroblast Activities
39	PP-39	Eva Dania Kosasih	Factors Affecting The Successful Treatment of Patients Pulmonary Tuberculosis New Cases and Tuberculosis Comorbid Diabetes Mellitus at Balai Besar Kesehatan Paru Masyarakat (BBKPM) Bandung
40	PP-40	Juni Ekowati	Docking Study of Ferulic Acid Derivatives on P2y12 Receptor and Their ADMET Prediction
41	PP-41	Mira Andam Dewi	Characterization Of Quinin Honey (*Cinchona succirubra*) Using ATR-FITR Combined With Chemometric
42	PP-42	Winasih Rachmawati	Docking Study and Toxicity Prediction of Plant Bioactive From Yacon Leaves (*Smallanthus sonchifolius*) As Alpha-Glucosidase Inhibitors

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ABSTRACT (OP-02)

Quantitative Structure-Activity Relationship (QSAR) of *N'*-ethyl-*N'*-phenyl-*N*-benzoylthiourea and Its Derivatives as Anticancer Compounds by *In Silico* Study

D. Kesuma[1*], Siswandono[2], H. Santosa [2]

[1] Department of Pharmaceutical Chemistry, Faculty of Pharmacy, University of Surabaya, Jalan Raya Kalirungkut, Surabaya 60293, Indonesia
[2] Department of Pharmaceutical Chemistry, Faculty of Pharmacy, University of Airlangga, Jalan Dharmawangsa Dalam, Surabaya 60286, Indonesia
Email: dinikesuma@gmail.com

Quantitative Structure Activity Relationship (QSAR) has important role in drug development that is improving efficiency on next research to determine new derivatives which are more potent, safer, and have good absorption when consumed. In this research we used *N'*-Ethyl-*N'*-Phenyl-*N*-Benzoylthiourea and 12 derivatives which have anticancer activity based on *in silico* test. Then, we conducted their relationship analysis of physicochemical properties (lipophilic, electronic, and steric) to *in silico* prediction of activity, toxicity, and bioavailability to obtain the best QSAR equation. QSAR equation was determined by linear and non linier regression using statistic program of SPSS 20.0. The result showed that activity prediction (Log 1/RS, from docking on RR receptor PDB ID: 2EUD) with the best QSAR equation: Log 1/RS = 0,118 Mw + 22,994 pKa + 0,022 $tPSA^2$ – 2,590 tPSA –270,960 (n = 13; R = 0,949; SE = 2,054; F = 18,150; Sig = 0,000), toxicity prediction (Log 1/LD-50, ACD/I-Lab prediction) with the best QSAR equation: Log 1/(LD-50 Mouse oral*)* = – 4,527 Mw – 0,496 $tPSA^2$ + 57,150 tPSA + 744,724 (n = 13; R = 0,925; SE = 61,569; F = 17,846; Sig = 0,000), and bioavailability prediction (Log1/F, ACD/I-Lab prediction) with the best QSAR equation: Log 1/F = – 0,006 Mw – 0,003 tPSA – 2,554 (n = 13; R = 0,802; SE = 0,132; F = 9,006; Sig = 0,006). Furthermore, all of the best equation can be used to develop new compounds as anticancer agent.

Keywords: anticancer, *in silico*, *N'*-ethyl-*N'*-phenyl-*N*-benzoylthiourea, QSAR