

## PHARMACEUTICAL

### A PRE SYNTHESIS STUDY : DOCKING, TOXICITY PREDICTION, AND PHARMACOPHORE IDENTIFICATION OF N-((4-FLUOROPHENYL) CARBAMOTHIOYL)BENZAMIDE SERIES AS SIRTUIN-1 INHIBITOR

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Department of Medicinal Chemistry, Faculty of Pharmacy, University of SurabayaIndonesia

#### ABSTRACT

Development anticancer drug targeted which has high activity and low toxicity is still promising. In silico method is possible to visually depict in three dimensions of the ligand (drug) and its receptors, predict toxicity, and identify pharmacophore. We have selected N-((4-Fluorophenyl) Carbamothioyl) Benzamide (NBFFT) series with three steps, Docking, toxicity, and pharmacophore prediction on cytotoxic activity in sirtuin-1. Method: we used Molegro Virtual Docker 5.5 for docking with sirtuin-1 receptors in protein data bank (4i5i.pdb), toxicity prediction by ProTox, and pharmacophore identification by LigandScout 4.3.2. Result: Docking result selected five active compounds compared with hydroxyurea; NBFFT15, NBFFT14, NBFFT19, NBFFT 13, and NBFFT17 from their low rerankscore. Then from toxicity prediction, four compounds eliminated and remained NBFFT13 with dimethylamine moiety. Last, NBFFT13 had several pharmacophore to strengthen their activity on sirtuin-1 amino acids receptor. Conclusion: NNBFFT13 is promising to continue synthesis and next step of drug development sirtuin-1 inhibitor.

**Key words: Docking, Toxicity, pharmacophore, N-((4-Fluorophenyl) Carbamothioyl) Benzamide**



# UMGESHIC 2020

Universitas Muhammadiyah Gresik  
Engineering, Social Science, and Health  
International Conference

## ABSTRACT BOOK

“ ENHANCING HUMAN RESOURCES PRODUCTIVITY  
THROUGH ENGINEERING, SOCIAL SCIENCE, AND HEALTH  
DURING COVID-19 PANDEMIC ”

DECEMBER 9 - 10, 2020 || GRESIK - INDONESIA

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LEMBAGA PENELITIAN DAN PENGABDIAN KEPADA MASYARAKAT  
UNIVERSITAS MUHAMMADIYAH GRESIK

**UMGESHC 2020 ABSTRACT BOOK**  
*Enhancing Human Resources Productivity through  
Engineering, Social, Science, and Health during  
Covid 19 Pandemic*

Penulis:

Nur Fauziyah  
Sukaris  
Andi Rahmad Rahim  
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Paulina  
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Indra Gita Anugrah

**Lembaga Penelitian dan Pengabdian Kepada  
Masyarakat  
Universitas Muhammadiyah Gresik**

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**Penulis:**

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Dilarang memperbanyak karya tulis ini dalam bentuk dan dengan Cara apapun tanpa ijin tertulis dari penerbit

## Kata Pengantar

Assalamualaikum Warahmatulla Hiwabarokatuh

Pertama-tama, marilah kita bersyukur kepada Allah SWT, Yang Maha Kuasa, atas berkah-Nya, karena membimbing kita ke jalan yang benar, dan karena telah memberikan kita semua sarana dan kesempatan bersama di sini untuk menghadiri acara yang penuh makna ini.

Atas Nama Universitas Muhammadiyah Gresik, kami sangat tersanjung dan senang menyambut Bapak / Ibu di *International Conference on Engineering, Social, Science and Health, University of Muhammadiyah Gresik (UMGESHC) 2020*. Kami juga ingin menyampaikan terima kasih kepada semua Keynote speaker yang telah menerima undangan kami untuk menjadi keynote speaker pada konferensi ini. Apresiasi juga kami sampaikan dan terima kasih kepada penyelenggara konferensi, co-host, semua reviewer, serta penulis atas kontribusinya dalam menyukseskan acara UMGESHIC 2020. Kami juga sangat mengapresiasi penerbitan kami, partner, IOP Publishing, atas dukungan kolaboratif mereka dalam menerbitkan prosiding konferensi.

Tujuan dari UMGESHIC 2020 adalah untuk memberikan beberapa peluang penelitian yang nantinya dapat diimplementasikan dan dikembangkan dalam kehidupan nyata, mengingat tantangan saat ini dalam Revolusi Industri 4.0, khususnya dalam Pengembangan Sumber Daya Manusia serta Teknologi Informasi. Melalui konferensi Internasional ini, kami ingin terlibat dengan Anda semua dalam dialog terbuka dan konstruktif tentang berbagai topik di bidang *Engineering, Social, Science and Health*. Apalagi wabah pandemi masih menjadi masalah yang menakutkan bagi hampir semua negara dan mempengaruhi semua aspek kehidupan manusia. Oleh karena itu, konferensi ini diharapkan dapat memberikan solusi atas permasalahan yang muncul.

Hadirin sekalian, akhirnya izinkan saya mengucapkan semoga Konferensi yang bermanfaat dan menyenangkan bagi Anda. Semoga acara ini sukses dan membawa kita lebih banyak ilmu dan manfaat kedepannya.

Gresik, Februari 2021

Rektor Universitas Muhammadiyah Gresik.

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## Message from the Rector

Assalamualaikum Warahmatulla Hiwabarokatuh

First of all, let us thank Allah SWT, the Almighty, for His blessing, for guiding us into the right path, and for granting us all means and opportunities together here to attend this meaningful occasion. On behalf of the University of Muhammadiyah Gresik, we are greatly honored and pleased to welcome you to Universitas Muhammadiyah Gresik Engineering, Social, Science and Health International Conference (UMGESHC) 2020. We would also like to extend our gratitude to all Keynote speakers who have accepted our invitation to become the invited keynote speakers of this conference. We would also like to give our appreciation and thank you to the conference organizers, co-host, all of the reviewers, as well as the authors for their contribution to making the success of the event of UMGESHIC 2020. We also greatly acknowledge our publishing partner, IOP Publishing, for their collaborative support in publishing the conference proceedings. The goal of UMGESHIC 2020 is to provide some research opportunities which can later be implemented and developed in the real-life, given the current challenges in this Industrial Revolution 4.0, especially in Human Resource Development as well as Information Technology. Through this International conference, we would like to engage with all of you in an open and constructive dialogue about various topics on Engineering, Social, Science as well as Health. Moreover, the pandemic breakout is still a frightening issue for almost all countries and affects all aspects of human life. Therefore this conference, hopefully, can bring some solutions to the problems arise from this. Ladies and gentlemen, finally allow me to wish you a fruitful and pleasant Conference. May this event be successful and bring us more knowledge and benefits in the future.

Wassalamualaikum Warahmatulla Hiwabarokatuh

Rector University of Muhammadiyah Gresik  
**Prof. Dr. Ir. Setyo Budi, M.S.**

## Acknowledgment

Assalamualaikum warahmatulla Hiwabarokatuh

My name is Andi Rahmad Rahim, chairman of the 2020 series 1th UMGESHIC committee. Thank you for the opportunity given. All praise is due to Allah, the Lord of the World, the Master and the Creator of everything in the Universe, the Destroyer of all oppressors and the Hope of the oppressed, for enabling us to meet together in this UMGESHIC (Universitas Muhammadiyah Gresik Engineering, Social Science and Health International Conference). Peace and salutation be upon the noble Prophet of Islam, Muhammad S.A.W. and his household, companions, and faithful followers until the end of time. The honorable, The Rector, and the entire academic community of the University of Muhammadiyah Gresik. The honorable, all first and second-day keynote speakers and plannery session. Those who are willing to share their knowledge at this international conference.

I want to say thank you very much to the entire committee of the international conference who had hard work to prepare this conference with good, and especially to all the Participants and Presenter of this International Conference. This international conference's theme is "Enhancing Human Resources Productivity through engineering, social science, and health during covid -19 Pandemic." This international conference talks about increasing human resources' productivity as an example of human performance to remain productive during the Covid-19 pandemic in engineering, social science, and health. At this conference, we will get much important information. Therefore, I, who represent all the committee, hope that this conference can be useful. That was the opening remarks on the second day.

Wassalamualaikum Warahmatulla Hiwabarokatuh

Chairman of the Confrence

**Dr. Andi Rahmad Rahim, S.Pi, M.Si.**

## **Committee**

**Conference Chair:**

Dr. Andi Rahmad Rahim, S.Pi, M.Si.

**Committees**

Dr. Nur Fauziah, S.Pd. M.Pd.  
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### Keynote Speakers

**Michael Lumintang Loe, dr, M.Si, M.Ked (Neusurg), Sp, BS, FINPS**

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#### Educational Background

- Post Graduate Doctoral Program, Medical Faculty, University.
  - Neurosurgery Residency, Universitas Sumatera Utara.
- Master Program, Medical Faculty, Universitas Sumatera Utara.
- Master Program, Medical Faculty, Airlangga University, Surabaya
- Medical Doctor, Medical Faculty, Brawijaya University, Malang

#### Organization membership

- American Association of Neurological Surgeons (AANS)
  - European Association of Neurosurgical Societies
    - Congress of Neurological Surgeons -US
      - PERSPEBSI
  - Fellow of Indonesian Neurosurgical Pain Society

#### International medical training

- 2019 - Neurosurgery Dept. Mayo Clinic Jacksonville, US
- 2017 - Fujita Health University, Nagoya, Aichi, Japan

### **Rusly Harsono**

Clinical Assistant Professor, Pediatrics - Critical Care

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- Pediatric Critical Care Medicine

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- Clinical Assistant Professor, Pediatrics - Critical Care

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**Nariman Salih Ahmad, Ph.D**

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Education and Qualifications: March 2013 Ph. D. in Plant Biotechnology (Molecular Genetics and Breeding), School of Biosciences the University of Nottingham, UK Dissertation: Genetic analysis of plant morphology in Bambara groundnut (*Vigna subterranea* L. (Verdc.)) November 2003 M.Sc. in plant breeding University of Sulaimani, Iraq Thesis: Diallel crossing and genetic analysis of some tobacco varieties. July 1997 B. Sc. In Agronomy University of Sulaimani, Iraq Current Work: ▪ Academic staff (Assistant Professor) at the Department of Biotechnology and Crop Science, College of Agricultural Engineering Sciences, University of Sulaimani, Kurdistan-Iraq ▪ Project Manager at Kurdistan Botanical Foundation <http://kurdistanbotanical.org/>, Sulaimani- Iraq. ▪ Editorial Board of the Journal of Life and Bio-Sciences Research (JLBSR) with ISSN: 2708-1818, <https://jlbsr.org/index.php/jlbsr>. Employee History: ▪ Assistant professor at the University of Sulaimani, College of Agricultural Engineering Sciences from Dec. 2015 until now. ▪ Lecturer at the University of Sulaimani, University of Sulaimani, College of Agricultural Engineering Sciences, from June 2007 until Dec. 2015. ▪ Assistant lecturer at the University Of Sulaimani College Of Agricultural Engineering Sciences, from Jan 2004 until May 2007. ▪ M Sc. Student at the University of Sulaimani College of Agricultural Engineering Sciences, from October 2001 until Nov. 2003.

**Tito G. Vivas-Buitrago, M.D, PhD**

Dr. Vivas-Buitrago's project with the lab's basic neurosurgery research team focuses on neurogenesis in the subventricular zone and the role it plays in brain cancer throughout its development and progression. He also works on emerging technology translation to the surgical and academic fields.

As part of the clinical neurosurgery team, he is helping elucidate the behavior of remnant glioblastoma cells after surgical resection in the recurrence of brain lesions and has assisted in the development of the neurosurgical textbook "Video Atlas of Neurosurgery: Contemporary Tumor and Skull Base Surgery."

Dr. Vivas-Buitrago first joined Dr. Quinones-Hinojosa's team for six months in 2014 as a medical student finishing his last subinternship rotation. He did part of his subinternship at the Naval Force Hospital in Cartagena, Colombia, and the Comuneros Hospital in Bucaramanga, Columbia. He received his medical degree from the University of Santander in Bucaramanga in 2014. He is funded by the Universidad de Santander, Colombia, and the Neurotrauma Center I.P.S., Bucaramanga, Colombia.

## Conference Program

**UMGESHC 2020**  
**9 - 10 December 2020**

### Agenda Day 1, Wednesday, 9 December 2020

Time Schedule	Events	PIC
07.00 - 08.00	Registration	Committee
08.00 - 08.05	Opening and welcoming dance	MC
08.05 - 08.20	Singing Indonesian National Anthem	MC, Operator
	Indonesia Raya	
	Singing Mars Muhammadiyah	
	Sang Surya	
08.20 - 08.25	Welcoming Speech	MC, Rector
08.25 - 08.30	Speech: Vice Rector I	Vice Rector I
08.30 - 12.30	<b>Enhancing Human Resources Productivity on Engineering, Social, Science, and Health during Covid 19 Pandemic</b>	Keynote Speakers, Moderator
	Speakers:	
08.30 - 09.00	1. Rusly Harisono, MD., MBA., M.Sc., FAAP - Stanford University, California US	
09.00 - 09.30	2. Tito Vivas-Butrago, MD., Ph.D. - Mayo Clinic, Florida US.	
09.30 - 10.00	3. Nariman Salih Ahmad, Ph.D. - University of Sulaiman Iraq	
10.00 - 10.30	<b>- DISCUSSION</b> <b>- Certificate Awarding</b>	
10.30 - 11.00	4. Dr. Hasimah Ja'afar - University Pendidikan Sultan Idris Malaysia	
11.00 - 11.30	5. Pregiwati Pusporini, Ph.D- University of Muhammadiyah Gresik Indonesia	
11.30 - 12.00	<b>- DISCUSSION</b> <b>- Certificate Awarding</b>	
12.00 - 13.00	<b>BREAK</b>	
13.00 - 15.00	Parallel Session	Moderator



**Agenda Day 2, Thursday, 10 December 2020**

<b>Time Schedule</b>	<b>Events</b>	<b>PIC</b>
07.15 - 08.15	Registration	Committee
08.15 - 08.20	Opening	MC
08.20 - 08.30	Welcoming Speech	MC, Chairman of the Committee
08.30 - 12.30	<b>Enhancing Human Resources Productivity on Engineering, Social, Science, and Health during Covid 19 Pandemic</b>	Speakers, Moderator
	Speakers:	
08.30 - 09.00	1. Dr. Anidah Binti Robani - Universiti Teknikal Malaysia Melaka Malaysia	
09.00 - 09.30	2. Sumar Hendrayana, Ph.D. – Universitas Pendidikan Indonesia	
09.30 -10.00	3. dr. Michael Lumintang Loe, M.Si., M.Ked (Neusug), Sp. BS., FINPS – Post Graduate Doctoral Program, Universitas Airlangga / Siloam Hospital Palangka Raya	
10.00 -10.30	<b>- DISCUSSION</b> <b>- Certificate Awarding</b>	
10.30 -11.00	4. Siti Maesurri Patahudin, Ph.D. – University of Canberra Australia	
11.00 -11.30	5. Al-Ghaliya Humaid Khamis Al Mamari, Ph.D.-Sultanate of Oman.	
11.30 – 12.00	<b>- DISCUSSION</b> <b>- Certificate Awarding</b>	
12.00 - 13.00	<b>BREAK</b>	Committee
13.00 - 15.00	Parallel Session	Moderator Class
15.00 - 15.30	Closing Remark	MC, Rector

## Pararel Sessions 1

### Day 1 Wednesday, 9 December 2020

<b>Moderator (Economi)</b>	<b>Dr. Moh. Agung SURIANTO, S.E., M.S.M.</b>
<b>Bussienes Manajemnt</b>	
Anita Handayani, Dewi Ayu Gandini	Mediating Effects of Capital Structure in the Financial Performance Manufacturer Company in Indonesia
Fandi Prasetya	The response of Micro, Small and Medium Enterprises in the face of the Corona Virus Diseases (COVID-19) Pandemic situation
Fani Sarika, Suryani Murad	Retailer's Strategy in Reshaping Consumers' Satisfaction and Wellbeing during a Pandemic
<b>Accounting</b>	
Nyimas Wardatul Afiqoh	Good University Governanceto Improvestudent Service And Trust (Study At the University Of Muhammadiyah Gresik)
Sasya Sabrina, Chandra Wijaya, Edwin Hendra	The Effect of Book-Tax Conformity, Investment Opportunity Set, and Audit Quality on Earnings Response Coefficient
Armanto Witjaksono, Yudistira Yudatama	The Influence of Professional Skepticism, Independence, Competence, and Experience on Auditor's Ability to Detectfraud
<b>Entrepreneurship</b>	
Beni Dwi Komara, Laily, Heri Cahyo Bagus Setiawan, Aries Kurniawan	Illage Community Business in Maintaining Traditional Food "Opak Ladu" Based On Creative Economics
Vembri Aulia Rahmi, Nanang Bagus Setiawan, Hadi Ismanto	Business Sustainability of Village Product in Gresik, Indonesia
Heri Cahyo Bagus Setiawan, Aries Kurniawan, Beni Dwi Komara	Implementation of Theory Z William Ouchi in Pesantrenpreneur: Study on Organizational Culture
<b>Moderator (Engineering)</b>	<b>Muhammad Zainuddin FATHONI, S.T., M.MT.</b>
<b>Engineering</b>	
Ade Ariesmayana, Ismiyati, M. Kosasih	the influence of coagulant al <sub>2</sub> so <sub>4</sub> and pac (poly alumunium chloride) toward leachate water quality tpa cilowong based enviromental standard
Choirul Anam, Benny Arif Pambudiarto, Zainal Mustakim, Fiska Yohana Purwaningtyas	Deproteination process on the chitin isolation from placuna placenta shells
Herry Purnama, Nurhadyati	Utilization Of Red Dragon Fruit Extract On

	The Dye Sensitized Solar Cell (Dssc) Application With The Touchscreen Capacitive Layer
<b>Industrial</b>	
Efta Dhartikasari Priyana, Pressa Perdana Surya Saputra.	Alternative Selection of Study Programs In Faculty of Engineering Based On 4 Criteria With Statistical Approach And Technique For Order Performance By Similary To Ideal Solution
Dzakiyah Widyaningrum	Performance Measurement Framework for Aquaculture Supply Chain Performance: Weighting Criteria by Unity
Moh. Dian Kurniawan, Iksan	Recommending Supply Chain Management Performance Improvement Using The Scor (Supply Chain Operations Reference) Methodat Pt Polowijo Gosari Gresik
<b>Moderator (Law)</b>	<b>Dr. Nirwanto Ma'ruf, SS., M.Hum.</b>
Dodi Jaya Wardana, Sukardi, Radian Salman	Instruments Of Democracy In Law-Making In Indonesia
Erna Ratnaningsih, Siti Yuniarti	The Limitation of the Right to Assembly and the Right to Movement in Order to Fulfil the Rights to Health of Society in the Covid-19 Pandemic in Indonesia
Nirmala Many, Muhammad Reza Syariffudin Zaki and Cecilia Elisabeth Agatha	Marine Casualty Caused By Ever Judger In Balikpapan Bay, Human Error Or Technical Factors
Austin Al Hariz, Nashriana, Vera Novianti	Legal Protection for Child Victims of Violence in Primary School
Iron Sarira	Justice as the Aim of/for Formation of Labor Law in Indonesia (A Review of Philosophy of Law)
<b>Moderator (Health)</b>	<b>Noviatul Rochmah, S.Pd., M.Pd.</b>
Diyan Indriyani, Asmuji, Triawan Adi Cahyanto, Astrid Maharani, Sri Wahyuni.	Community empowerment through independent family health evaluation (IFHE)-based healthy villages
Wahyu Dewi Sulistyarini, Siti Mukharomah	Psychometric Testing and Cross-Cultural Adaptation of the Indonesian version of The Short Form Survivor Unmet Needs Survey (SF-SUNS)
Siti Sopiaturun, Sri maryati	The Influence Of Posyandu Cadre Training On Knowledge And Attitudes In Efforts To Prevent Stunting In Karawang

## Pararel Sessions 2

### Day 2 Thursday, 10 December 2020

<b>Moderator (Islamic Study)</b>	<b>Ribeh Najib Muhammad, S.Pd., M.Pd.</b>
Mohammad Ahyan Yusuf Sya'bani	Culture Of Religious Moderation Through The Actualization Of Islamic Education Wasatiyyah To Improve Religious Reconnection And Tolerance In Indonesia
Tika Widiastuti, Muryani, Puji Sucia Sukmaningrum,	Critical Review of Social Safety Net in COVID Era Based On Maqashid Sharia Framework: Indonesia Case
Sukron Ma'mun, Ramot Peter, Catarina Manurung.	The Improvement of Understanding and Tolerance Attitude of Binus Students through Character Education
Taqiyah Dinda Insani, Tika Widiastuti, Anidah Robani, Rahmat Yuliawan	E-Reporting of Islamic Bank in Indonesia: Enhancing Productivity in Pandemic Covid-19
Imron Mawardi, Sri Ningsih, Wisudanto, Tika Widiastuti <sup>4</sup> , Muhammad Ubaidillah Al Mustofa, Anidah Robani.	Efficiency Analysis of Indonesian Islamic Microfinance Institution: Case of East Java
<b>Moderator (Education)</b>	<b>Riska Widyanti Batubara, S.Hum., M.Pd.</b>
Nuansa Bayu Segara, Agus Suprijono, Katon Galih Setyawan	Designing Measurement Model Of Self Determined Learning During The Covid-19 Pandemic
T Y Ardiyansah, R W Batubara P K Auliya	Pre-Service Teachers' Satisfaction Towards Online Learning Process In International Internship Program In Thailand
Ribeh Najib Muhammad, Paulina	Lecturers' Resistance To Implementing Distance Learning
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Rahmad Jumadi, Suhaili, Wiharyanti Nur Lailiyah.	Growth and yield of several sorghum (sorghum bicolor (L.) Moench) Varieties Using Seed Biomatriconditioning Treatment
S. Budi	Study of Several Superior Sugarcane Clones

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U Firmani, R Nurdiani, A W Ekawati and H Nursyam.	Gut bacteria community of the milkfish (Chanos chanos Forskal.) in Gresik, East Java Province
Sri Wiyatiningsih, Wiwik Sri Harijani, Wahyu Santoso, Riko Setya Wijaya, and Khoirur Rojikin.	Biopesticide Applications To Improve The Resistance Of Pummelo Orange Plant (Citrus Maxima) Against Diplodia Disease (Botryodiplodia Theobromae Path.)
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<b>Moderator (Psychology)</b>	<b>Awang Setiawan Wicaksono, S.Psi. M.Psi.</b>
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