

**LEMBAR
HASIL PENILAIAN SEJAWAT SEBIDANG ATAU PEER REVIEW
KARYA ILMIAH : PROSIDING**

Judul Karya Ilmiah : Ab Initio Computational Study of Electronic Structure Part-1: Reaction Mechanism of Peptide Bond Formation Between Amino Acid Alanine and Glycine

Jumlah Penulis : 4 Orang

Status Pengusul : Penulis ke-4

Identitas Prosiding : a. Judul Prosiding : Journal of Physics: Conference Series: The 8th Internasional Seminar on New Paradigm and Innovation on Natural Sciences and Its Application (INSPINSA) 2018

b. ISBN/ISSN : 978-1-5108-6265-4 / 1757-8981

c. Thn Terbit, Tempat Pelaks. : 2019, Semarang – Indonesia

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Alamat Artikel : <https://iopscience.iop.org/article/10.1088/1742-6596/1217/1/012053>

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- Ruang lingkup dan kedalaman pembahasan:** Penulis dapat mendiskripsikan penelitian mengenai sifat elektronik molekul yang terlibat dalam reaksi sintesis peptide. Para penulis juga membahas mengenai mekanisme reaksi sintesis pembentukan ikatan peptide antara asam amino alanin dan glisin pada empat jalur mekanisme reaksi serta mampu membuktikan mekanisme reaksi yang lebih disukai dengan menggunakan pendekatan komputasi ab initio. Pada artikel ini kita dapat mengetahui mekanisme reaksi yang terjadi hingga ke tingkat elektron.
- Kecukupan dan kemutakhiran data/informasi dan metodologi:** Informasi yang disajikan dalam artikel tersebut cukup untuk menjelaskan mekanisme reaksi yang lebih disukai pada sintesis pembentukan ikatan peptide antara alanin dan glisin dari empat jalur mekanisme. Juga, metode perhitungan komputer yang digunakan mutakhir dan sangat akurat dan terdapat gambar serta grafik yang membantu untuk memahami isi artikel ilmiah tersebut. Terdapat referensi sebanyak 23 artikel (7 artikel terbit 10 tahun terakhir) menandakan bahwa telah dilakukan studi literatur yang baik. Beberapa referensi yang digunakan tidak tertuliskan dengan baik.
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Semarang, 10 April 2023

Reviewer 1

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Prof. Dr. Dwi Hudyanti, M.Sc

NIP. 19650622 198903 2 001

Unit Kerja : Kimia FSM Undip

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a. Kelengkapan unsur isi prosiding (10%)	3,00		3,00
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Catatan Penilaian Paper oleh Reviewer :

- Kesesuaian dan kelengkapan unsur isi paper:** Unsur jurnal sudah lengkap, meliputi; Judul, Abstrak, Pendahuluan, Metode, Hasil dan Pembahasan, Kesimpulan, dan Referensi. Daftar referensi sebanyak 23 literatur yang sudah bereputasi. Setiap bab dalam artikel saling terkait satu sama lain dengan penjelasan yang cukup jelas, sesuai dengan kaidah penulisan ilmiah yang baik dan benar.(3)
- Ruang lingkup dan kedalaman pembahasan:** Penulis membahas mengenai mekanisme yang terjadi pada pembentukan ikatan peptida antara asam amino alanin dan glicine dengan metode komputasi abinitio. Mekanisme yang terjadi pada dua asam amino tersebut akan membentuk dua produk Ac-AG-NH₂ dan Ac-AG-NH₂, dengan empat jalur mekanisme yang memungkinkan, sementara antara glisin dengan glisin yang menghasilkan produk Ac-GG-NH₂ dengan dua jalur mekanisme yang memungkinkan digunakan sebagai pembandingan. Pendekatan penulis yang dilakukan untuk menentukan reaksi mana yang dapat berjalan adalah dengan perhitungan energi aktivasi, reaksi yang disukai adalah reaksi dengan energi aktibasi yang rendah, sehingga reaksi mampu bejalan lebih cepat. Penjabaran mekanisme reaksi yang dilakukan oleh penulis dengan kajian ilmu komputasi dapat dijelaskan setiap langkahnya secara lengkap dan urut. Perhitungan-perhitungan yang dilakukan sangat lengkap sehingga mampu diterapkan sebagai studi awal ketika akan melakukan eksperimen empiris di laboratorium. Penyajian data penelitian sangat menarik dan mudah untuk dibaca, dengan data pendukung literatur yang bereputasi. Pembahasan yang dilakukan oleh penulis sangat sistematis.(9)
- Kecukupan dan kemutakhiran data/informasi dan metodologi:** Informasi serta data yang ditampilkan dalam artikel ini sangat lengkap dan jelas dengan penjabaran yang mudah dipahami. Selain itu, referensi yang digunakan merupakan jurnal internasional yang bereputasi, dengan kajian komputasi yang mutakhir. Hanya 3 dari 23 referensi bersumber dari artikel ang terbit 5 tahun atau sebelumnya (13%) (8)
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Semarang, 25-3-2021

Reviewer 2

A handwritten signature in black ink, consisting of a stylized 'M' followed by a cursive 'C' and 'D'.

Prof. Dr. Muhammad Cholid Djunaidi, S.Si., M.Si

NIP 19700702 199603 1 004

Unit Kerja : Kimia FSM Undip

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Hasil Penilaian *Peer Review* :

Komponen Yang Dinilai	Nilai Reviewer		Nilai Rata-rata
	Reviewer I	Reviewer II	
a. Kelengkapan unsur isi prosiding (10%)	3,00	3,00	3,00
b. Ruang lingkup dan kedalaman pembahasan (30%)	9,00	9,00	9,00
c. Kecukupan dan kemutakhiran data/informasi dan metodologi (30%)	8,00	9,00	9,00
d. Kelengkapan unsur dan kualitas terbitan/prosiding(30%)	8,00	8,00	8,00
Total = (100%)	28,00	29,00	28,50
Nilai Pengusul = (40% x 28,50) = 11,40			

Semarang, 10 April 2023

Reviewer 2



Prof. Dr. Muhammad Cholid Djunaidi, S.Si., M.Si
NIP 19700702 199603 1 004
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Reviewer 1



Prof. Dr. Dwi Hudyanti, M.Sc
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Ab initio computational study of electronic structure part-1: Reaction mechanism of peptide bond formation between amino acid alanine and glycine

Dzikrullah A.^a; Cahyono B.^b; Laksitorini M.D.^c; Siahaan P.^a

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^a Physical Chemistry Laboratory, Department of Chemistry, Faculty of Sciences and Mathematics, Diponegoro University, Semarang, Indonesia

^b Organic Chemistry Laboratory, Department of Chemistry, Faculty of Sciences and Mathematics, Diponegoro University, Semarang, Indonesia

^c Department of Pharmaceutics, Faculty of Pharmacy, Gadjah Mada University, Sekip Utara, Yogyakarta, Indonesia

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Yuliani, S.V. , Salimah, S.N.M. , Hudiyan, D.
(2019) *Journal of Physics: Conference Series*

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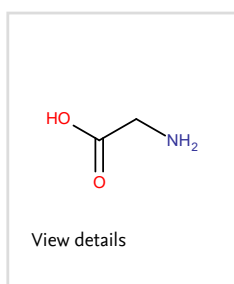
Abstract

The porosity of the peptide delivery pathway to the brain is hindered by the presence of tight junctions which are intercellular cadherin interactions, but this can be overcome by modulating the cadherin molecule using peptide derived synthesis, one of which is ADT-10 (Ac-QGADTPVGV-NH₂)' where there are amino acids glycine (G) and alanine (A). Formation reaction of the peptide is one of the most important chemical reactions, one way to probe the reaction of peptide synthesis is the computational method. The purpose of this research is to determine which mechanism of the reaction is most preferred to the synthesis of peptide bond formation between alanine and glycine from four pathways of the reaction mechanism, as well as glycine and glycine from two pathway of reaction mechanisms by ab initio computational approach. The calculations were carried out by theory and basis set HF/6-31g**. The results show the most preferred reaction of peptide synthesis of amino acid glycine and alanine is on the mechanism IV which result in Ac-GA-NH₂ with activation energy 759.614 kJ·mol⁻¹, while in glycine and glycine is on the mechanism II with an activation energy of 933.550 kJ·mol⁻¹. © Published under licence by IOP Publishing Ltd.

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The 8th International Seminar on New Paradigm and Innovation on Natural Science and Its Application

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Abstract

The 8th International Seminar on New Paradigm and Innovation on Natural Sciences and Its Application (ISNPINSA-8) is annual seminars organized by Faculty of Sciences and Mathematics (FSM) Diponegoro University and has been successfully conducted since 2011. The ISNPINSA-8 was held in Semarang, Indonesia on September 26th 2018. The aims of ISNPINSA are to facilitate brain storming and state of the art information in field of sciences and mathematics; to increase innovation of technology that can be applied in industries; to contribute in formulating strategy to increase the role of science for community; and to stimulate collaboration between industries, researchers and government to increase community welfare. The theme of 8th ISNPINSA in 2018 is "*Science and Applied Science for Sustainable Development Goals*".

The number of participants of the seminar were 272 including keynote speakers, invited speakers, oral presenters, poster presenters, and non presenters coming from various institutions of various countries, including Japan, Philippines, Thailand, Malaysia, Australia, Bangladesh, China, Kazakhtan, Vietnam

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