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

Judul Karya Ilmiah	:	Ab Initio Computational Study of Reaction Mechanism of Peptide Bond Formation on HF/6-31G(d,p) Level		
Jumlah Penulis	:	5 Orang		
Status Pengusul	:	Penulis ke-1		
Identitas Prosiding	:	a. Judul Prosiding	:	IOP Conference Series: Materials Science and Engineering: 11th Joint Conference on Chemistry in Conjunction with the 4th Regional Biomaterials Scientific Meeting
		b. ISBN/ISSN	:	978-1-5108-6265-4 / 1757-8981
		c. Thn Terbit, Tempat Pelaks.	:	2017, Purwokerto - Indonesia
		d. Penerbit/Organiser	:	IOP Publishing Ltd
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		Alamat Artikel	:	https://iopscience.iop.org/article/10.1088/1757-899X/172/1/012040
		f. Terindeks di (jika ada)	:	Scopus/Scimagojr/SJR = 0,2 (2019)

Kategori Publikasi Makalah (beri ✓pada kategori yang tepat) : [√] *Prosiding* Forum Ilmiah Internasional
[ ] *Prosiding* Forum Ilmiah Nasional

Hasil Penilaian *Peer Review* :

Komponen Yang Dinilai	Nilai Maksimal Prosiding		Nilai Akhir Yang Diperoleh
	Internasional [ ]	Nasional [ ]	
a. Kelengkapan unsur isi prosiding (10%)	3,00		3,00
b. Ruang lingkup dan kedalaman pembahasan (30%)	9,00		9,00
c. Kecukupan dan kemutahiran data/informasi dan metodologi (30%)	9,00		8,00
d. Kelengkapan unsur dan kualitas terbitan/prosiding(30%)	9,00		8,50
Total = (100%)	**30,00**		**28,50**
Nilai Pengusul = (60% x 28,50) = 17,10			

Catatan Penilaian Paper oleh Reviewer :

1. **Kesesuaian dan kelengkapan unsur isi paper:** Pembahasan artikel saling terkait sesuai kaidah penulisan ilmiah yang baik dan benar dengan penjelasan yang jelas. Unsur-unsur jurnal sudah lengkap meliputi Judul, Abstrak, Pendahuluan, Metode, Hasil dan Pembahasan, Kesimpulan dan Daftar Pustaka.
2. **Ruang lingkup dan kedalaman pembahasan:** Penulis dapat mendeskripsikan penelitian mengenai sifat elektronik dari molekul yang terlibat dalam mekanisme reaksi pembentukan ikatan peptide pada sintesis Ac-PV-NH2 dan Ac-VP-NH2 dari asam amino. Penulis juga mampu menunjukkan mekansisme reaksi yang paling disukai dari empat jalur mekanisme reaksi pembentukan ikatan peptida pada sintesis Ac-PV-NH2 dan Ac-VP-NH2 dari asam amino prolin dan valin melalui pendekatan komputasi secara ab initio. Pada artikel ini, kita dapat mengetahui keadaan transisi (*transition state*) pada tiap jalur mekanisme reaksi yang cukup sulit diperoleh secara eksperimental.
3. **Kecukupan dan kemutakhiran data/informasi dan metodologi:** Informasi yang disajikan dalam artikel cukup untuk menjelaskan mekanisme reaksi yang terjadi pada pembentukan ikatan peptide pada sintesis Ac-PV-NH2 dan Ac-VP-NH2 dari asam amino dan mengkonfirmasi reaksi yang paling disukai dari empat jalur mekanisme reaksi tersebut melalui energi aktivasi yang diperoleh, serta terdapat gambar dan grafik yang membantu untuk memahami isi artikel. Juga, metode perhitungan komputer yang digunakan mutakhir dan sangat akurat. Terdapat referensi sebanyak 23 artikel (11 artikel terbit 10 tahun terakhir). menandakan bahwa telah dilakukan studi literatur yang baik.
4. **Kelengkapan unsur dan kualitas terbitan:** IOP Publishing Ltd sudah berindeks scopus dengan nilai SJR 0,2 (2017). Similarity index berdasarkan Turnitin adalah 8% sehingga memiliki orisinalitas baik

Semarang, 10 April 2023

Reviewer 1

Prof. Dr. Dwi Hudiyanti, M.Sc
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Unit Kerja : Kimia FSM Undip

LEMBAR
HASIL PENILAIAN SEJAWAT SEBIDANG ATAU *PEER REVIEW*
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		c. Thn Terbit, Tempat Pelaks.	:	2017, Purwokerto - Indonesia
		d. Penerbit/Organiser	:	IOP Publishing Ltd
		e. Alamat Repository/Web	:	https://iopscience.iop.org/issue/1757-899X/172/1
		Alamat Artikel	:	https://iopscience.iop.org/article/10.1088/1757-899X/172/1/012040
		f. Terindeks di (jika ada)	:	Scopus/Scimagojr/SJR = 0,2 (2019)

Kategori Publikasi Makalah (beri ✓pada kategori yang tepat) : [√] *Prosiding* Forum Ilmiah Internasional
[ ] *Prosiding* Forum Ilmiah Nasional

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 kemutahiran data/informasi dan metodologi (30%)	8,00	8,00	8,00
d. Kelengkapan unsur dan kualitas terbitan/prosiding(30%)	8,50	9,00	9,00
Total = (100%)	**28,50**	**29,00**	**28,75**
Nilai Pengusul = (60% x 28,75) = 17,25			

Semarang, 10 April 2023

Reviewer 2

Prof. Dr. Muhammad Cholid Djunaidi, S.Si., M.Si
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Unit Kerja : Kimia FSM Undip

Reviewer 1

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Unit Kerja : Kimia FSM Undip

LEMBAR
HASIL PENILAIAN SEJAWAT SEBIDANG ATAU *PEER REVIEW*
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		f. Terindeks di (jika ada)	:	Scopus/Scimagojr/SJR = 0,2 (2019)

Kategori Publikasi Makalah (beri ✓pada kategori yang tepat) : [√] *Prosiding* Forum Ilmiah Internasional
[ ] *Prosiding* Forum Ilmiah Nasional

Hasil Penilaian *Peer Review* :

Komponen Yang Dinilai	Nilai Maksimal Prosiding		Nilai Akhir Yang Diperoleh
	Internasional [ ]	Nasional [ ]	
a. Kelengkapan unsur isi prosiding (10%)	3,00		3,00
b. Ruang lingkup dan kedalaman pembahasan (30%)	9,00		9,00
c. Kecukupan dan kemutahiran data/informasi dan metodologi (30%)	9,00		8,00
d. Kelengkapan unsur dan kualitas terbitan/prosiding(30%)	9,00		9,00
Total = (100%)	**30,00**		**29,00**
Nilai Pengusul = (60% x 29) = 17,4			

Catatan Penilaian Paper oleh Reviewer :

1. **Kesesuaian dan kelengkapan unsur isi paper:** Paper untuk prosiding lengkap, terdiri dari pendahuluan, metode komputasi, hasil dan pembahasan, kesimpulan dan referensi. Referensi 90% berasal dari jurnal internasional bereputasi. Setiap bab mampu menjelaskan bab sebelumnya dan saling terkait satu sama lain. (3)
2. **Ruang lingkup dan kedalaman pembahasan:** Artikel membahas tentang studi komputasi mekanisme reaksi yang terjadi pada pembentukan ikatan peptida dari asam amino proline dan valine. Kepentingan dari penelitian dijabarkan oleh penulis dengan baik yaitu mengenai *Blood brain barrier* yang sulit untuk dilewati oleh obat-obatan yang akan masuk ke bagian dalam otak karena adanya interaksi cadherin-chaderin antar sel, satu-satunya cara adalah melalui interaksi jalur paraseluler (dalam artikel ini, memodulasi protein cadherin dengan sintesis turunan peptida cadherin). Penulis mampu memodelkan mekanisme reaksi beserta energi yang diperlukan dalam pembentukan ikatan peptida dari asam amino prolin dan valin. Terdapat 4 jalur antara reaktan dan keadaan transisi (1, 2, 3, dan 4), penulis mampu mengusulkan sintesis Ac-PV-NH_2 dan Ac-VP-NH_2 dari asam amino prolin dan valin paling bereaksi pada jalur 1 yang diinisiasi dengan H^+ melalui perhitungan komputasi abinitio yang memiliki tingkat akurasi tinggi. Berdasarkan pembahasan tersebut, penulis mampu menjabarkannya dengan baik dan runtut. Namun Figur 7 tidak ada dan Figure 8 tidak disitasi di dalam artikel (8)
3. **Kecukupan dan kemutakhiran data/informasi dan metodologi:** Penyajian data dalam artikel cukup untuk menjelaskan interaksi yang terjadi dalam sintesis ikatan peptida dari asam amino prolin dan valin. Metode perhitungan komputasi yang digunakan juga mutakhir dan memiliki tingkat akurasi yang tinggi. Rujukan dalam penyajian data berasal buku dan jurnal yang bereputasi.Hampir separoh (50%) referensi merupakan artikel yang terbit 5 tahun atau sebelumnya (9)
4. **Kelengkapan unsur dan kualitas terbitan:** IOP Publishing adalah perusahaan penerbitan Institute of Physics. Penerbit tersebut menyediakan publikasi melalui mana penelitian ilmiah didistribusikan di seluruh dunia, termasuk jurnal, situs web komunitas, majalah, proses konferensi dan buku. Pada artikel ini berupa terbitan prosiding oleh IOP Publishing yang sudah berindeks scopus dengan nilai SJR 0,2 (2019).

Turnitin: 16% dengan exclude quote dan bibliografi On.

Semarang, 25-03-2021

Reviewer 2

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IOP Conference Series: Materials Science and Engineering • *Open Access* • Volume 172, Issue 1 • 17 February 2017 • Article number 012040 • 11th Joint Conference on Chemistry, JCC 2016, in Conjunction with the 4th Regional Biomaterials Scientific Meeting • Purwokerto • 15 September 2016through 16 September 2016 • Code 126603

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Ab initio computational study of reaction mechanism of peptide bond formation on HF/6-31G(d,p) level

Siahaan P.[a] ; Lalita M.N.T.[a]; Cahyono B.[a]; Laksitorini M.D.[b]; Hildayani S.Z.[a]

Save all to author list

[a] Diponegoro University, Semarang, Indonesia

[b] Gadjah Mada University, Yogyakarta, Indonesia

Abstract

Peptide plays an important role in modulation of various cell functions. Therefore, formation reaction of the peptide is important for chemical reactions. One way to probe the reaction of peptide synthesis is a computational method. The purpose of this research is to determine the reaction mechanism for peptide bond formation on Ac-PV-NH_2 and Ac-VP-NH_2 synthesis from amino acid proline and valine by ab initio computational approach. The calculations were carried out by theory and basis set HF/6-

31G(d,p) for four mechanisms (path 1 to 4) that proposed in this research. The results show that the highest of the rate determining step between reactant and transition state (TS) for path 1, 2, 3, and 4 are 163.06 kJ.mol^{-1}, 1868 kJ.mol^{-1}, 5685 kJ.mol^{-1}, and 1837 kJ.mol^{-1}. The calculation shows that the most preferred reaction of Ac-PV-NH_2 and Ac-VP-NH_2 synthesis from amino acid proline and valine are on the path 1 (initiated with the termination of H^+ in proline amino acid) that produce Ac-PV-NH_2. © Published under licence by IOP Publishing Ltd.

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11th Joint Conference on Chemistry in Conjunction with the 4th Regional Biomaterials Scientific Meeting

IOP Conference Series: Materials Science and Engineering, Volume 172, 11th Joint Conference on Chemistry in Conjunction with the 4th Regional Biomaterials Scientific Meeting 15–16 September 2016, Purwokerto, Indonesia

Citation 2017 *IOP Conf. Ser.: Mater. Sci. Eng.* **172** 011001

DOI 10.1088/1757-899X/172/1/011001

Abstract

Welcome Message From Chairman of Conference

On behalf of the Committee, I am very pleased that the 11th Joint Chemistry Conference in Conjunction with The 4th Regional Biomaterials Scientific Meeting has attracted many scientist from Indonesia, Malaysia, Thailand, Bangladesh, Egypt, Japan as well as other countries.

This international conference is attended by more than 150 participants covering wide variety subject grouped as theoretical chemistry and educational, material synthesis and modification, bioscience and analysis, and also Industrial and environmental chemistry. The given oral and poster presentation would showing outputs for future need as indicated in the conference theme of "Material Chemistry Development for Future Medicine, Industry, Environmental and Biomaterial Application"

The success of the Conference would not have been attained without strong supports from contributing scientists and our partner institutes including Diponegoro University, Semarang State University, Sebelas Maret University, Satya Wacana Christian University and Indonesian Biomaterial Society. I would like to thank all of them for helping to make a very successful conference.

Chairman,

Amin Fatoni, Ph.D

Committee

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Amin Fatoni, Ph.D (*Universitas Jenderal Soedirman, Indonesia*)

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Accepted papers received: 25 January 2017
Published online: 17 February 2017

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Preface

Papers

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A Kartiwa, R Miraprahesti, I Sovani, S Enus and A Boediono

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Operculum bone carp (*cyprinus carprio sp*.) scaffold is a new potential xenograft material: *a preliminary study*

A Kartiwa, B Abbas, P Pandansari, A Prahasta, M Nandini, M Fadhlillah, T Subroto and R Panigoro

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