

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

Judul Karya Ilmiah : Ab-Initio Computational Study of Noncovalent Interaction between Peptide and Alkaline Metal Ions on HF/6-31 G** Level

Jumlah Penulis : 5 Orang

Status Pengusul : Penulis ke-1

Identitas Prosiding : a. Judul Prosiding : AIP Conference Proceedings: The 3rd International Seminar on Chemistry (ISoC) 2018: Green Chemistry and its Role for Sustainability

b. ISBN/ISSN : 978-0-7354-1775-5

c. Thn Terbit, Tempat Pelaks. : 2018, Surabaya - Indonesia

d. Penerbit/Organiser : AIP Publishing LLC

e. Alamat Repository/Web : <https://aip.scitation.org/toc/apc/2049/1>

Alamat Artikel : <https://aip.scitation.org/doi/10.1063/1.5082458>

f. Terindeks di (jika ada) : Scopus/Scimagojr/SJR = 0,19 (2019)

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

Hasil Penilaian *Peer Review* :

Komponen Yang Dinilai	Nilai Maksimal Prosiding		Nilai Akhir Yang Diperoleh
	Internasional <input type="checkbox"/>	Nasional <input type="checkbox"/>	
a. Kelengkapan unsur isi prosiding (10%)	3,00		3,00
b. Ruang lingkup dan kedalaman pembahasan (30%)	9,00		8,5
c. Kecukupan dan kemutakhiran data/informasi dan metodologi (30%)	9,00		8,5
d. Kelengkapan unsur dan kualitas terbitan/prosiding(30%)	9,00		9,00
Total = (100%)	30,00		29
Nilai Pengusul = (60% x 29) = 17,4			

Catatan Penilaian Paper oleh Reviewer :

- 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 buku dan jurnal internasional bereputasi. Setiap bab mampu menjelaskan bab sebelumnya dan saling terkait satu sama lain (3)
 - Ruang lingkup dan kedalaman pembahasan:** Pembahasan dalam artikel didasarkan pada bidang ilmu kimia komputasi, yaitu mempelajari interaksi nonkovalen yang terjadi antar peptida cadherin dengan ion K⁺, dan Na⁺ melalui perhitungan ab-initio. Kepentingan penelitian telah dijelaskan dengan baik oleh penulis, terkait dengan *blood-brain barrier*. Cakupan yang dibahas dalam artikel ini secara lengkap dijabarkan oleh penulis dengan baik, yaitu struktur peptida sistein-alanin dan valin-sistein dengan perhitungan komputasi abinitio; stabilitas interkasinya dengan K⁺ dan Na⁺, bahkan penulis juga dapat memberi penjelasan mengenai kontribusi muatan parsial dan energi HOMO-LUMO dari interaksi peptida dengan K⁺ dan Na⁺. Pendekatan ilmu komputasi yang dijelaskan oleh penulis dapat menjadi rujukan untuk dilakukan secara eksperimen empiris. Penjelasan tabel 2 dan 3 kurang lengkap terutama efek sterik tidak dijelaskan lebih detail (8,5)
 - Kecukupan dan kemutakhiran data/informasi dan metodologi:** Penyajian data dalam artikel cukup untuk menjelaskan interaksi yang terjadi dalam sintesis ikatan peptida dari asam amino sistein-alanin dan valin-sistein. Metode perhitungan komputasi yang digunakan juga mutakhir dan memiliki tingkat akurasi yang tinggi. Rujukan dalam penyajian data berasal buku dan jurnal yang bereputasi. Lebih dari 50% referensi yang digunakan adalah artikel yang terbit 5 tahun atau sebelumnya. Namun ada dua referensi tanpa nama jurnal ataupun informasi selain tahun (8,5)
 - Kelengkapan unsur dan kualitas terbitan:** AIP Conference Proceedings merupakan serial yang diterbitkan oleh American Institute of Physics (AIP) sejak 1970. Ini menerbitkan prosiding dari berbagai konferensi bidang fisika. AIP Publishing telah menjadi sumber terpercaya jurnal penelitian, prosiding konferensi, dan informasi penting bagi ilmuwan fisika di mana pun, dengan indeks scopus dan nilai SJR = 0.19 (2019). (9)
- Turnitin:** 9% dengan exclude quote dan bibliografi On.

Semarang, 26-03-2021

Reviewer 1

Prof. Dr. Muhammad Cholid Djunaidi, S.Si., M.Si
NIP 19700702 199603 1 004
Unit Kerja : Kimia FSM Undip

LEMBAR
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- f. Alamat Artikel : <https://aip.scitation.org/doi/10.1063/1.5082458>
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Kategori Publikasi Makalah : *Prosiding* Forum Ilmiah Internasional
(beri ✓ pada kategori yang tepat) *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		
b. Ruang lingkup dan kedalaman pembahasan (30%)	8,5		
c. Kecukupan dan kemutahiran data/informasi dan metodologi (30%)	8,5		
d. Kelengkapan unsur dan kualitas terbitan/prosiding(30%)	9,00		
Total = (100%)	29		
Nilai Pengusul = (60% x) =			

Semarang,

Reviewer 2

Reviewer 1

Prof. Dr. Meiny Suzery, MS
NIP. 196005101989032001
Unit Kerja : Kimia FSM Undip

Prof. Dr. Muhammad Cholid Djunaidi, S.Si., M.Si
NIP 19700702 199603 1 004
Unit Kerja : Kimia FSM Undip

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	Internasional <input type="checkbox"/>	Nasional <input type="checkbox"/>	
a. Kelengkapan unsur isi prosiding (10%)	3,00		3,00
b. Ruang lingkup dan kedalaman pembahasan (30%)	9,00		8,50
c. Kecukupan dan kemutakhiran data/informasi dan metodologi (30%)	9,00		8,50
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 :

- Kesesuaian dan kelengkapan unsur isi paper:** Kelengkapan unsur isi jurnal telah terpenuhi karena pada artikel tersebut terdapat pendahuluan, metode, hasil dan pembahasan, kesimpulan dan referensi. Setiap unsur isi jurnal berkaitan satu sama lain. Artikel tersebut sesuai pedoman penulisan karya ilmiah. Serta referensi yang dijadikan acuan pada artikel ilmiah ini 90% berasal dari jurnal yang bereputasi.
- Ruang lingkup dan kedalaman pembahasan** Artikel ini berisi tentang interaksi interaksi peptida Ac-CA-NH₂ dan Ac-VC-NH₂ dengan K⁺ dan Na⁺ dengan pendekatan komputasi ab initio. Pembahasan dalam artikel dijelaskan dengan cukup detail oleh penulis, di mulai dari optimasi geometri, energi interaksi hingga analisis HOMO LUMO yang dapat menjelaskan sifat elektronik pada interaksi peptida dengan K⁺ dan Na⁺. Penulis juga memvisualisasikan interaksi antara peptida dengan K⁺ dan Na⁺ dalam bentuk gambar sehingga dapat membantu memahami hasil yang diperoleh pada artikel.
- Kecukupan dan kemutakhiran data/informasi dan metodologi:** Penelitian telah menghasilkan data/informasi yang berkaitan sehingga dapat saling menjelaskan. Metodologi yang diuraikan mudah untuk dipahami. Data yang tersaji dalam prosiding sudah cukup untuk menjelaskan struktur sistein-alanin dan valin-sistein serta interaksi peptida Ac-CA-NH₂ dan Ac-VC-NH₂ dengan ion kalium dan natrium. Metode komputasi yang digunakan juga mutakhir. Pada artikel ini, data/informasi dan metodologi sudah cukup dan mutakhir karena telah menyertakan referensi dari jurnal ilmiah bereputasi. Namun terdapat dua referensi yang tidak tertera nama jurnal maupun informasi lainnya selain tahun terbit.
- Kelengkapan unsur dan kualitas terbitan:** Artikel ini sudah memenuhi kualitas terbitan karena diterbitkan oleh AIP Conference Proceedings adalah serial yang diterbitkan oleh American Institute of Physics (AIP). Program conference proceeding ini melaporkan temuan yang dipresentasikan dalam pertemuan ilmiah dalam konferensi internasional besar hingga spesialis lokakarya kecil. AIP Publishing menjadi sumber terpercaya prosiding konferensi dan jurnal penelitian. Selain itu memberikan penerbitan yang cepat dengan indeks scopus dan nilai SJR = 0.18 (2018)

Semarang, 12 April 2023

Reviewer 2

A handwritten signature in blue ink, appearing to read 'M. Suzery', with a horizontal line underneath.

Prof. Dr. Meiny Suzery, MS
NIP. 196005101989032001
Unit Kerja : Kimia FSM Undip

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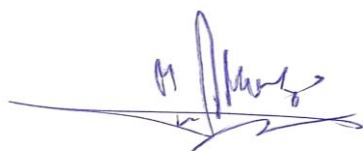
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	Reviewer I	Reviewer II	
a. Kelengkapan unsur isi prosiding (10%)	3,00	3,00	3,00
b. Ruang lingkup dan kedalaman pembahasan (30%)	8,50	8,50	8,50
c. Kecukupan dan kemutahiran data/informasi dan metodologi (30%)	8,50	8,50	8,50
d. Kelengkapan unsur dan kualitas terbitan/prosiding(30%)	9,00	8,50	8,50
Total = (100%)	29,00	28,50	28,75
Nilai Pengusul = (60% x 28,75) = 17,25			

Semarang, 12 April 2023

Reviewer 2



Prof. Dr. Meiny Suzery, MS
NIP. 196005101989032001
Unit Kerja : Kimia FSM Undip

Reviewer 1



Prof. Dr. Muhammad Cholid Djunaidi, S.Si., M.Si
NIP 19700702 199603 1 004
Unit Kerja : Kimia FSM Undip



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Ab-initio computational study of noncovalent interaction between peptide and alkaline metal ions on HF/6-31 G** level

Siahaan, Parsaoran^a ; Christian, Rinaldy^a; Fauziah, Anisa Nur^a; Hudiyantri, Dwi^a; Prasasty, Vivitri Dewi^b

Save all to author list

^a Departement of Chemistry, Faculty of Science and Mathematics, Diponegoro University, Indonesia

^b Faculty of Biotechnology, Atma Jaya Catholic University of Indonesia, Indonesia

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Interaction of Phospholipid, Cholesterol, Beta-Carotene, and Vitamin C Molecules in Liposome-Based Drug Delivery Systems: An in Silico Study

Hudiyantri, D. , Putri, V.N.R. , Hikmahwati, Y. (2023) *Advances in Pharmacological and Pharmaceutical Sciences*

Computational study: Noncovalent interaction of cyclic peptide with alkaline earth metal ions and its conformation changes

Tresnoningtiyas, M.A. , Nurwarrohman, A.S. , Ihyar, K. (2021) *Key Engineering Materials*

Probing the interaction between EC1-EC2 domain of E-cadherin with conformational structure of cyclic ADTC7 (Ac-CDTPDC-NH2) peptide using molecular docking approach

Siahaan, P. , Darmastuti, N.E. , Aisyafalah, S. (2020) *Journal of Physics: Conference Series*

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Improving in vivo brain delivery of monoclonal antibody using novel cyclic peptides

Ulapane, K.R. , Kopec, B.M. , Siahaan, T.J. (2019) *Pharmaceutics*

Abstract

Intermolecular interaction or non-covalent interaction plays an important role on the chemical processes. Intermolecular interaction also involves several phenomena that corresponding to molecular and macromolecular sciences. Intermolecular interaction phenomena become an important subject to be learned because they can explain the important process on the human body. One of the most important processes that can be learned is peptide-metal ion interaction. Peptide-metal ion interaction plays the important role for the biological process on the human body. One of the peptide-metal ion interaction that can be learned is cadherin peptide interaction with a metal ion on blood-brain barrier (BBB). Several methods were done for investigating peptide-metal ion interaction. Generally, peptide-metal ion interaction can be investigated experimentally and theoretically. The purpose of this research is to theoretically determine the structure of Ac-CA-NH₂ (Cysteine-Alanine) and Ac-VC-NH₂ (Valine-Cysteine) peptides by ab initio computational approach with a minimum energy; the interaction stability of Ac-CA-NH₂ and Ac-VC-NH₂ with potassium and sodium ions, respectively; and to understand the contribution of partial charge and Highest Occupied Molecular Orbital (HOMO) - Lowest Unoccupied Molecular Orbital(LUMO) energy on Ac-CA-NH₂ and Ac-VC-NH₂ peptide interaction with potassium and sodium ions. The calculations were carried out on HF/6-31G** including geometry optimization of peptides, geometry optimization of peptide-ion interaction, and physical and chemical properties determination such as partial charge and HOMO-LUMO energy. The results show that the most stable structure of Ac-CA-NH₂ and Ac-VC-NH₂ peptides were acquired with minimum energy -965.254 Hartree and -1043.320 Hartree, respectively, proven by their optimization convergences. The interaction energy of Ac-CA-NH₂ with sodium and potassium ion indicating the most stable configurations-1 with interaction energy -189,782 kJ/mol for sodium ion and -141.280 kJ/mol for potassium ion. Meanwhile, the interaction energy of Ac-VC-NH₂ peptide with sodium and potassium ions has the most stable configuration-1 with interaction energy -248,562 kJ/mol and -181,022 kJ/mol, respectively. The partial charge and HOMO-LUMO energy can be used for understanding the stability of peptide-metal ion interaction and also confirming the reactivity of the peptide after interacting with a metal ion. © 2018 Author(s).

Author keywords

Ab-initio; alkaline metal ion; drug interaction; non-covalent interaction; peptide

SciVal Topics 

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Funding details


References (42)


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Probing of interaction mode between linear and cyclic ADTC6 (Ac-CDTPPC-NH₂) with E-cadherin protein using molecular docking approach

Siahaan, P., Kaswanda, J.A., Budiyanto, R.

(2019) *IOP Conference Series: Materials Science and Engineering*

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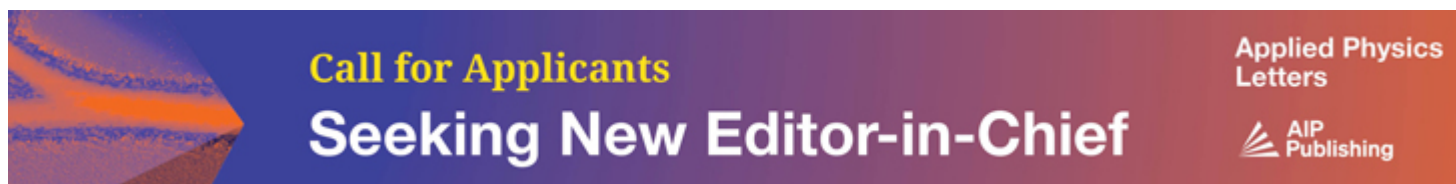
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